TVD Flux-Difference Split Methods for High-Speed Thermochemical Nonequilibrium Flows with Strong Shocks

by

Clinton P. T. Groth

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Abstract

This study is concerned with the numerical solution of high-speed nonequilibrium gaseous flows with strong shocks. The extension of modern total-variation-diminishing (TVD) shock-capturing schemes to include thermochemical nonequilibrium high-temperature effects is of primary interest. Partially-decoupled upwind-based TVD flux-difference split schemes for the solution of the conservation laws governing two-dimensional nonequilibrium vibrationally relaxing and chemically reacting flows of thermally-perfect gaseous mixtures are presented. Both time-split semi-implicit and factored implicit flux-limited TVD upwind schemes are described. The semi-implicit formulation is more appropriate for unsteady applications whereas the factored implicit form is useful for obtaining steady-state solutions. As well, a multigrid version of the fully implicit TVD scheme is also proposed for the more efficient computation of time-invariant solutions. The multigrid algorithm is based on the full approximation storage (FAS) and full multigrid (FMG) concepts and employs the partially-decoupled factored implicit scheme as the smoothing operator in conjunction with a four-level V-cycle coarse-grid-correction procedure.

In the proposed methods, a novel partially-decoupled flux-difference splitting approach is adopted. The fluid conservation laws and the finite-rate species concentration and vibrational energy equations are decoupled by means of a frozen flow approximation. The resulting partially-decoupled gas dynamic and thermodynamic subsystems are then integrated alternately in lagged manner within a two-stage time marching procedure, thereby providing explicit coupling between the two equations sets. Extensions of Roe's approximate Riemann solvers, giving the eigenvalues and eigenvectors of the fully coupled systems, are used to evaluate the numerical flux functions. Additional modifications to the Riemann solutions are also described which ensure that the approximate solutions are not aphysical. Moreover, concerns associated with the satisfaction of monotonicity, positivity, and maximum principles are addressed. The proposed partially-decoupled methods are shown to have some computational advantages over chemistry-split and fully coupled techniques in coping with large systems of equations with stiff source terms.

The predictive capabilities of the shock-capturing methods are demonstrated and their usefulness appraised, by solving a number of different flows with both complicated shock structure and complex nonlinear wave interactions. The problems considered include nonstationary oblique shock-wave reflections and diffractions and steady high-speed nozzle, compression ramp, and blunt-body flows. The numerical results are compared to available experimental data in many cases.
Acknowledgments

The author would like to express his sincere gratitude and appreciation to the thesis supervisor Professor J. J. Gottlieb for providing encouragement, guidance, and friendship throughout the course of this work. The author is also grateful for having had the opportunity of studying at the University of Toronto Institute for Aerospace Studies (UTIAS) and would like to acknowledge all of the friends, students, and staff at UTIAS for making the doctoral research program both intellectually rewarding and enjoyable.

The author's gratitude also goes to his wife, Annette Hansen, for all her help in proofreading the various drafts of the thesis. As well, the useful discussions with Professors J. P. Sislian, P. A. Sullivan, and D. W. Zingg are very much appreciated. Thanks are also given to Mr. R. L. Deschambault and Mr. V. Pugliese of UTIAS for helping to reproduce the experimental data.

Finally, the author would like to express a special thanks to his family for all of their encouragement and supportive actions.

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Nomenclature

Roman Symbols

\( a \)  
\text{sound speed}

\( A \)  
\text{cross-sectional area of duct}

\( A \)  
\text{source term column vector}

\( \dot{A} \)  
\text{Jacobian of \( \zeta \)-direction flux vector \( \hat{F} \)}

\( b \)  
\text{antidiffusive flux ratio}

\( \dot{B} \)  
\text{Jacobian of \( \eta \)-direction flux vector \( \hat{G} \)}

\( C_s \)  
\text{species mass fraction}

\( C^f_s \)  
\text{forward reaction rate coefficient for reaction \( r \)}

\( C^b_r \)  
\text{backward reaction rate coefficient for reaction \( r \)}

\( C_p \)  
\text{specific heat at constant pressure}

\( D_a \)  
\text{Damköhler number}

\( D_h \)  
\text{hydraulic diameter}

\( e \)  
\text{total specific internal energy}

\( e_{tr} \)  
\text{translational-rotational energy of mixture}

\( e_v \)  
\text{vibrational energy}

\( e_{vs} \)  
\text{specific vibrational energy of species \( s \)}

\( e_{vs}^0 \)  
\text{equilibrium specific vibrational energy of species \( s \)}

\( e^\nu \)  
\text{eigenvectors of homogeneous flux vector Jacobian}

\( E^f_r \)  
\text{activation energy for forward reaction \( r \)}

\( E^b_r \)  
\text{activation energy for backward reaction \( r \)}

\( f \)  
\text{Darcy-Weisbach friction factor}

\( F_p \)  
\text{frictional force acting on the piston}

\( F_{wall} \)  
\text{equivalent wall boundary-layer viscous body force}

\( F_{loss} \)  
\text{equivalent pressure-loss body force}

\( F \)  
\text{\( \zeta \)-direction flux column vector}

\( \hat{F} \)  
\text{homogeneous flux column vector (Appendix B)}

\( \hat{G} \)  
\text{\( \zeta \)-direction flux column vector of gas dynamic subsystem}

\( \hat{G} \)  
\text{\( \eta \)-direction flux column vector}

\( \hat{G} \)  
\text{\( \eta \)-direction flux column vector of gas dynamic subsystem}

\( h \)  
\text{total specific energy of mixture}

\( \Delta h^0_f, \)  
\text{heat of formation of species \( s \)}

\( H \)  
\text{flux column vector of thermodynamic subsystem}

\( I \)  
\text{light intensity}

\( I \)  
\text{identity matrix}

\( J \)  
\text{Jacobian of coordinate transformation}

\( J \)  
\text{Jacobian of homogeneous flux vector (Appendix B)}

viii
\( k \)  
thermal conductivity

\( k_f^r \)  
reaction rate of forward reaction \( r \)

\( k_b^r \)  
reaction rate of backward reaction \( r \)

\( k^q_r \)  
equilibrium constant of reaction \( r \)

\( K \)  
Boltzmann's constant

\( \mathcal{K} \)  
specific refractivity

\( \text{Kn} \)  
Knudsen number

\( L \)  
reference length

\( L_p \)  
piston length

\( m_p \)  
piston mass

\( M \)  
Mach number

\( \text{Ma} \)  
Mach number (Appendix B)

\( \mathcal{M} \)  
molecular weight

\( n \)  
refractive index

\( n_f^r \)  
forward reaction rate coefficient for reaction \( r \)

\( n_b^r \)  
backward reaction rate coefficient for reaction \( r \)

\( N \)  
total number of species in mixture

\( N_p \)  
total number of nodes in the discretized domain

\( N_R \)  
total number of elementary reactions

\( \text{Nu} \)  
Nusselt number

\( p \)  
pressure

\( \text{Pr} \)  
Prandtl number

\( q_s \)  
time rate of change of vibrational energy of species \( s \)

\( Q_{\text{wall}} \)  
wall heat transfer rate

\( Q_{\text{zero}} \)  
rate of change of mixture zero-point energy

\( Q \)  
conserved solution column vector of thermodynamic subsystem, nonequilibrium flow source term column vector (Appendix B)

\( r \)  
duct radius

\( r_p \)  
piston radius

\( R \)  
specific gas constant

\( R_s \)  
specific gas constant of species \( s \)

\( \mathcal{R} \)  
universal gas constant

\( R \)  
Reynolds number

\( R_p \)  
piston Reynolds number

\( S \)  
source term column vector

\( \dot{S} \)  
source term column vector of thermodynamic subsystem

\( t \)  
time

\( T \)  
temperature

\( T \)  
translational-rotational temperature

\( T_{vs} \)  
vibrational temperature of species \( s \)

\( u \)  
\( x \) component of velocity

\( U \)  
contravariant velocity component

\( U \)  
conserved solution column vector

\( v \)  
\( y \) component of velocity

\( V \)  
contravariant velocity component

\( V_p \)  
piston velocity

\( w_s \)  
time rate of change of concentration of species \( s \)
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<tr>
<td>$W$</td>
<td>conserved solution column vector of gas dynamic subsystem, nonequilibrium flow solution column vector (Appendix B)</td>
</tr>
<tr>
<td>$x$</td>
<td>horizontal coordinate of physical reference frame</td>
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<tr>
<td>$y$</td>
<td>vertical coordinate of physical reference frame</td>
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Greek Symbols

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<tr>
<td>$\alpha$</td>
<td>elemental wave strength</td>
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<td>$\beta$</td>
<td>flux limiter compression parameter</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>specific heat ratio</td>
</tr>
<tr>
<td>$\gamma_s$</td>
<td>frozen specific heat ratio of species $s$</td>
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<tr>
<td>$\epsilon$</td>
<td>entropy correction parameter, solution residual (Chapters 6 &amp; 7)</td>
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<td>$\zeta$</td>
<td>horizontal coordinate of computational reference frame</td>
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<td>$\eta$</td>
<td>vertical coordinate of computational reference frame</td>
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<td>$\theta$</td>
<td>spatial-differencing control parameter, flow deflection angle (Chapters 6 &amp; 7)</td>
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<tr>
<td>$\Theta$</td>
<td>time-stepping control parameter</td>
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<tr>
<td>$\Theta_{\nu,s}$</td>
<td>characteristic vibrational temperature of species $s$</td>
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<tr>
<td>$\lambda$</td>
<td>eigenvalues of homogeneous flux vector Jacobian, wavelength of light source (Chapter 6)</td>
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<td>$\Lambda$</td>
<td>compressibility correction factor</td>
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<td>$\mu$</td>
<td>dynamic viscosity</td>
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<td>$\nu$</td>
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<td>$\rho$</td>
<td>flow density</td>
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<td>$\sigma$</td>
<td>piston skirt porosity</td>
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<td>$\sigma^r_s, r$</td>
<td>stoichiometric coefficient of reactant species $s$ for reaction $r$</td>
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<td>$\sigma^b_s, r$</td>
<td>stoichiometric coefficient of product species $s$ for reaction $r$</td>
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<td>$\psi$</td>
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<td>$\omega$</td>
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<td>$\Omega$</td>
<td>time-stepping control parameter</td>
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Subscripts and Superscripts

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<td>$i$</td>
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<tr>
<td>$j$</td>
<td>index of spatial node of computational mesh</td>
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<td>$k$</td>
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<td>alternating-direction implicit</td>
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<td>MUSCL</td>
<td>monotonic upstream-centered scheme for conservation laws</td>
</tr>
<tr>
<td>NASA</td>
<td>National Aeronautics and Space Administration</td>
</tr>
<tr>
<td>NASP</td>
<td>National Aerospace Plane</td>
</tr>
<tr>
<td>PDE</td>
<td>partial-differential equation</td>
</tr>
<tr>
<td>PPM</td>
<td>piecewise parabolic method</td>
</tr>
<tr>
<td>RPI</td>
<td>Ryerson Polytechnical Institute</td>
</tr>
<tr>
<td>SOR</td>
<td>successive over relaxation</td>
</tr>
<tr>
<td>TVD</td>
<td>total-variation diminishing</td>
</tr>
<tr>
<td>UTIAS</td>
<td>University of Toronto Institute for Aerospace Studies</td>
</tr>
<tr>
<td>WAF</td>
<td>weighted average flux</td>
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</tbody>
</table>
Chapter 1

Introduction

1.1 Background

1.1.1 Hypersonic Aerodynamics

The rocketry and space exploration programs of the United States and former Soviet Union provided a strong impetus for research in hypersonics aerodynamics and aerophysics in the late 1950s and early 1960s. However, by the 1970s, these programs were drastically reduced and, in response to this, interest in hypersonics waned. Fifteen to twenty years later, during the mid to late 1980s, hypersonic aerodynamics experienced a significant world-wide revival. The increased research activity in this area was stimulated to a large extent by a number of major undertakings of the United States such as the National Aerospace Plane (NASP) initiative, the Aeroassisted Orbital Transfer Vehicle (AOTV) program, and the Personnel Launch System (PLS) project. European projects such as Hermes, Hotol, and Sänger, as well as the Japanese HOPE orbiting plane project, have also added greatly to the revival of hypersonic aerothermodynamic research. These and other national and international programs, coupled with additional interest in developing the next generation of high-speed civil transport (HSCT) for viable commercial use, have fostered research activity in all areas related to the design of advanced hypersonic transportation systems. The X-30 NASP, which is expected to be about 60 m in length and to have a gross weight of approximately 150,000 kg, is depicted in Figure 1.1.

The physics of hypersonic flow is significantly different from that of the subsonic, tran-
sonic, and supersonic regimes. By convention, *hypersonic flows* are generally assumed to be flows in which the free-stream Mach number $M$ is greater than five ($M > 5$). However, this classification is not precise. More precisely, the term refers to flows that are characterized by one or more of the following physical features which begin to appear at flow speeds far greater than the speed of sound [Anderson, 1984; Anderson, 1989]:

(i) **Thin Shock Layers.** At very high flow speeds, strong often oblique shocks form. The associated large increases in flow density permit the shock fronts to envelope and lie very close to a body positioned in the flow.

(ii) **Curved Shocks and Entropy Layers.** At the higher flow velocities, the shock waves also exhibit strong curvature and have varying strength (e.g., bow shock of blunt body). The curvature results in entropy gradients in the shock layers behind the shock front. The entropy layers are regions of strong vorticity and boundary layers immersed in these entropy layers can be difficult to analyze.

(iii) **High Temperatures.** At higher Mach numbers, the conversion of the high kinetic energy of the flow into internal or thermal energy through viscous dissipation within boundary layers or at stagnation points can create extremely high temperatures. These high temperatures can result in significant surface heating from diffusion, convection, and possibly radiation processes (in some cases, radiative heat transfer can account for a large portion of the total heating). Moreover, the temperatures may be severe enough to excite the internal vibrational energy modes and/or cause the dissociation of polyatomic molecules, and, if the temperature rise is sufficient, even ionize the gaseous molecules. For example, atmospheric re-entry temperatures can reach 11,000 K. For air, vibrational excitation typically becomes important at temperatures above 600–800 K, dissociation of oxygen molecules begins at about 1,500–2,000 K, and ionization becomes significant once temperatures exceed 8,000 K [Vincenti and Kruger, 1975; Anderson, 1982; Anderson, 1989]. These so-called high-temperature or real-gas effects bring about a dramatic departure in the thermodynamic behaviour of the gas from that of the ideal. Ionization of air in the stagnation regions of re-entry vehicles can also lead to communication blackouts.

(iv) **Viscous Interaction.** The presence of the very high temperatures also causes increases in the gas viscosity and decreases in the flow density within boundary layers. Consequently, the boundary layers of high-Mach-number flows are quite thick. The added thickness provides a much greater interaction between the fully viscous boundary layer and the outer inviscid flow region, which, in most cases, means that conventional boundary layer analysis is invalid and cannot be used.

(v) **Rarefied Low-Density Flow Effects.** For high-speed flight at very high altitudes, the density of the ambient air is very low. At sufficiently high altitudes, the collision rates and mean free path of the gaseous molecules are such that the usual assumption of continuum flow is no longer appropriate and the Navier-Stokes equations do not apply. For space shuttle reentry, this occurs at altitudes above 92 km [Anderson, 1989]. Kinetic theory and the Boltzmann equation must be utilized to study free molecular flow regimes of rarefied gases.
(vi) Ablation and Catalytic Wall Effects. For high-temperature chemically reacting flows near solid boundaries, ablation of the surface due to high-temperature melting and enhancement of chemical reaction rates due to gas-surface interactions at catalytic walls are very important in defining surface heat transfer rates.

The occurrence of any of these physical features is what makes hypersonic flows distinct from the other flow regimes and each of the phenomena must be considered in the design of any advanced hypersonic transportation system, if the problems of surface heating and aerodynamic loading are to be properly addressed.

A complete review of hypersonic aerodynamic research is beyond the scope of this thesis work. The early hypersonic flow theory of the 1950s and 1960s is summarized for the most part in the excellent texts of Chernyi [1961] and Hayes and Probstein [1966]. Although many important analytical contributions were made during this period, much of the research was experimental in nature, and the book by Lukasiewicz [1973] provides a fairly thorough description of early laboratory facilities and experimental techniques related to hypersonics. The more recent text by Anderson [1989] provides an up-to-date introduction to the field. A flavour of current research issues and directions for the 1990s may be gained from the proceedings of the recent IUTAM Symposium on Aerothermochemistry of Spacecraft and Associated Hypersonic Flows [Brun et al., 1992].

1.1.2 Recent Hypersonic Research at UTIAS

Although considerable past research has been conducted in all areas related to high-speed gas dynamics at the University of Toronto Institute for Aerospace Studies (UTIAS), much of the recent hypersonic research at UTIAS has been related to an experimental program involving the UTIAS-Ryerson Polytechnical Institute (RPI) hypersonic impulse tunnel. The UTIAS-RPI facility is a short-duration blow-down experimental wind tunnel capable of producing high Mach number flows (M ≈ 8). See Appendix B for a brief description. A number of experimental projects have been undertaken related to improving the understanding of the fluid mechanics associated with scramjet inlets for hypersonic air-breathing flight vehicles such as the NASP [Sullivan et al., 1992].

One topic of the current UTIAS hypersonics research program involves experimental measurements of shock-wave boundary-layer interactions in the vicinity of convex corners [Hawboldt, 1992; Sullivan et al., 1992]. The understanding of these interactions is of particular importance to supersonic and hypersonic scramjet inlet design. Oblique (cancellation) shocks generated at the cowls of external compression inlets are invariably used to turn inlet flows into the combustor entrances of engines. As a result, shock boundary-layer interactions with possible flow separation occur near the inlet corners [van Wie et al., 1990]. This is illustrated in Figure 1.2. It is desirable to minimize flow separation in these cases.

Another aspect of the recent work has been to investigate the operation of the UTIAS-RPI impulse tunnel so as to establish the range of test section flow properties that may be achieved. This was done through an experimental calibration procedure [Deschambault et al., 1989; Sullivan et al., 1992] and a quasi-one-dimensional numerical study [Groth et al., 1991; Sullivan et al., 1992]. The numerical study of the impulse tunnel was carried out as part of the present work and is reported on in Appendix B.
1.2 Motivation for the Present Study

1.2.1 Long Term Goal: Numerical Study of Shock-Wave Boundary-Layer Interactions

The limitations of scaled ground-based experimental facilities [Hornung, 1988; Lukasiewicz, 1973] such as the UTIAS-RPI impulse tunnel, the advent and subsequent rapid development of high-speed digital computers, and the vast improvements in numerical solution algorithms have meant that computational fluid dynamics (CFD) has been a useful and will be an even more important design tool in hypersonic aerodynamics [White et al., 1987]. As White et al. [1987] point out, computational codes for the solution of supersonic and hypersonic flow through scramjet inlets are now in routine use. They also point out that, although significantly more complex, computational codes have also been developed for the solution of viscous chemically reacting flow in scramjet combustors and nozzles.

The motivation for the present thesis stems from some long term goals to develop a suitable numerical algorithm and associated computer code for predicting two-dimensional planar and axisymmetric viscous hypersonic continuum flows of air and, subsequently, to use the CFD code as a tool for the investigation of shock-wave boundary-layer interactions for hypersonic laminar flows of air over flat plates and at concave and convex corners. This future numerical study will be conducted with a view to enhancing the physical understanding flow features such as separation, reattachment, and surface heating so as to aid in improving scramjet inlet design. It will complement the ongoing UTIAS experimental program dealing with hypersonic shock-wave boundary-layer interactions discussed in the previous subsection. An important aspect of the CFD work will be to address the significance of equilibrium and nonequilibrium high-temperature effects, such as dissociation/recombination, vibrational relaxation, and ionization, on the interactions.

1.2.2 Starting Point: Development of Two-Dimensional Inviscid Thermochemical Nonequilibrium Flow Solvers

High-resolution, robust, and efficient CFD algorithms capable of solving large systems of conservation laws with often stiff source terms are required to predict high-speed continuum viscous flows predominated by strong shock waves, high temperatures, and thermochemical nonequilibrium processes, such as vibrational relaxation, dissociation and recombination, and ionization. Therefore, a first step toward achieving the stated long-term research goals concerning hypersonic viscous flow solution has been to begin with the less complicated, but still challenging, inviscid non-ionized case; to restrict the attention to two-dimensional planar flows; and to develop sophisticated, reliable, and accurate solution algorithms and associated computational code for predicting time-dependent and steady inviscid compressible high-speed flows of gaseous mixtures that are in both thermal and chemical nonequilibrium (i.e., nonequilibrium vibrationally relaxing and chemically reacting flows). This dissertation reports on the above mentioned first step. The aim here is to devise computationally efficient schemes for high-speed flows characterized by strong shocks and nonequilibrium phenomena utilizing some of the more successful and powerful nonlinear solution techniques. Later work will involve extensions of the methods to the fully viscous, ionized, and axisymmetric flow cases and the computation of hypersonic shock-wave boundary-layer interactions.
1.3 Scope of the Present Study

1.3.1 Finite-Difference Based Upwind TVD FDS Schemes

As noted, the computation of high-speed continuum flows characterized by strong shocks and nonequilibrium phenomena is of concern in the present numerical study. In the last 10–15 years, progress in the design of modern finite-difference and finite-volume techniques has led to the development of several high-resolution nonoscillatory shock-capturing methods for numerically solving the nonlinear partial differential equations (PDEs) governing multidimensional flows with shocks. The total-variation-diminishing (TVD) concept of Harten [1983; 1984] and flux-difference-splitting (FDS) technique of Roe [1981] have both proven to be very useful in coping with the difficulties associated with computing discontinuous (generalized or weak) solutions to initial boundary value problems (IBVPs) of PDEs. This thesis describes both time-split semi-implicit and factored fully implicit upwind-biased TVD FDS finite-difference based schemes that have been adapted for the solution of the conservation laws for two-dimensional nonequilibrium vibrationally relaxing and chemically reacting flows of thermally-perfect gaseous mixtures. The proposed semi-implicit formulation is more appropriate for unsteady applications whereas the factored implicit form is useful for obtaining steady-state solutions via a time-marching approach. In addition, as multigrid methods [Brandt, 1977] have been shown to be very powerful and efficient solution techniques for boundary-value problems of linear and nonlinear PDEs, a multigrid version of the fully-implicit upwind TVD method is also considered for the more rapid solution of the steady flow equations. The presentation includes details of these solution algorithms, especially those particulars that are peculiar to the solution of the nonequilibrium flow equations. The computational techniques are validated by comparison to available experimental data.

It is reiterated that the inclusion of nonequilibrium finite-rate vibrational relaxation and chemical reaction effects in computationally efficient TVD solution algorithms is the present focus. Therefore, the study has been restricted to two-dimensional planar inviscid flows and ionization effects are neglected. Extensions of the methods for application to axisymmetric and three-dimensional viscous high-speed flows with ionization are possible and are potential topics of future research.

1.3.2 Outline of the Thesis

The organization of the thesis is as follows. A review of both classical and modern shock-capturing difference schemes is given in the next chapter, Chapter 2. This review includes a brief introduction to some of the important concepts of TVD methods and discusses and compares some of the more popular shock-capturing techniques that have been successfully adapted for the solution of high-speed nonequilibrium flow problems. The review is followed by a presentation in Chapter 3 of the conservation equations that are of interest: the nonlinear hyperbolic PDEs describing inviscid two-dimensional thermochemical nonequilibrium, as well as equilibrium, continuum gaseous flows. Chapter 4 is then concerned with providing complete and comprehensive descriptions of the proposed semi-implicit and fully implicit TVD FDS algorithms for solving these governing compressible flow equations. Included are details of the temporal and spatial discretization procedures, flux-difference splitting techniques and related approximate Riemann solvers, and treatment of the inhomogeneous terms. The proposed multigrid version of the fully implicit algorithm is outlined in Chapter 5. Example numerical predictions of these various methods using a five-species, four-temperature, nonequilibrium, thermodynamic model for air are described in Chapter
Chapter 7. In these chapters, numerical results are given for nonstationary oblique shock-wave reflection and diffraction problems in both air and pure oxygen, as well as the steady flow of air and pure nitrogen over a blunt-body, a compression ramp, and through a diverging nozzle. For some of these flows, comparisons are also given to experimental data obtained from the literature. A discussion of the results along with a few conclusions follow in Chapter 8. This chapter includes a summary of what is felt are the major contributions of the dissertation and some recommendations for future work.

It should also be mentioned that additional information is given in the four appendices regarding: 1) Roe-type approximate Riemann solvers for the proposed FDS methods; 2) the five-species four-temperature nonequilibrium model for air used in the example calculations; 3) a two-dimensional numerical grid generation technique that was used to obtain the curvilinear grids used in all of the two-dimensional computations; and 4) a related study concerning the use of the proposed nonstationary flow solver for the prediction of quasi-one-dimensional nonequilibrium flows in the UTIAS-RPI hypersonic impulse tunnel.
Figure 1.1: X-30 National Aerospace Plane (NASP). Schematic and picture courtesy of the NASP program.
Generic Scramjet Engine Inlet

- Cowl
- Combustor Entrance
- Developing Boundary Layer
- Shock-Isonropic Compression
- Inlet Ramp
- Shock-Wave Boundary-Layer Interaction

Figure 1.2: Schematic diagram of generic scramjet engine inlet.
Chapter 2

Review of Shock-Capturing Methods for Gas Dynamics

2.1 Introductory Remarks

As explained in Chapter 1, the existence of strong curved shocks with large density gradients is one of the distinctive characteristics of the hypersonic flow environment. In general, the numerical computation of weak solutions to flow problems with strong discontinuities, such as shocks, necessitates special consideration. This chapter provides a short review from a historical perspective of solution techniques for high-speed compressible flows with shocks, along with a discussion of the adaptation of these methods for flows undergoing chemical reactions, vibrational relaxation, and/or ionization, which are the concern of the present study. The proposed upwind TVD FDS methods for thermochemical nonequilibrium flows with shocks are then briefly previewed.

Note that much of the material on the basic theory of shock-capturing techniques that is reported here can be found elsewhere, such as in the excellent texts by Anderson et al. [1984] and Hirsch [1989; 1990], and in the reviews by Roe [1986a] and Moretti [1987]. However, relevant material is summarized herein for the sake of completeness. Note also that this review is by no means exhaustive. The focus is on finite-difference based methods and many techniques such as solution-adaptive node-moving finite-element and finite-difference methods [Hawken et al., 1991] are not discussed.

2.2 Hyperbolic Conservation Laws in One Space Dimension

For the purposes of the review discussion, it is convenient to consider initial value problems (IVPs) of one-dimensional quasi-linear hyperbolic conservation laws having the form

\[ \frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0, \quad u(x,0) = u_0(x), \]

(2.1)

defined on the semi-infinite domain \( D \) given by \( t \in [0, \infty) \) and \( x \in (-\infty, \infty) \). Here \( u(x, t) \) is the solution, which may be a scalar or vector (i.e., multi-component) quantity, \( f \) is the flux, and \( x \) and \( t \) are the spatial and temporal independent variables, respectively. It can be shown that this scalar or system of PDEs is strictly hyperbolic if the eigenvalues of the flux Jacobian \( A = \frac{\partial f}{\partial u} \) are all real (repeated values are permitted) and a complete set of distinct eigenvectors for the Jacobian can be defined.

Many physical phenomena, such as gas-dynamical flows, can be modeled by hyperbolic
PDEs of the form of Eq. (2.1) or multi-dimensional versions thereof. A genuine or regular solution of Eq. (2.1) is one that satisfies the PDEs and is Lipschitz continuous (i.e., \( u \) is \( C^0 \) with bounded discontinuities permitted in its derivatives \( \partial u / \partial t \) and \( \partial u / \partial x \)). However, hyperbolic conservation laws are invariably derived for the purposes of describing various physical systems and are therefore often related to integral forms of the associated conservation properties. Thus, in the general case, solutions to IVPs of the form of Eq. (2.1) are not necessarily continuous and differentiable. Even for continuous or smooth initial data \( u_0 \), the solution \( u \) can develop discontinuities within a finite time interval [Lax, 1973].

Although the PDEs would appear to be invalid for discontinuous solutions, it is possible to show that generalized or weak solutions of Eq. (2.1) are permitted that possess measurable and bounded discontinuities or shocks.\(^1\) These generalized solutions satisfy the conservation laws and are adequately differentiable everywhere (i.e., weak solutions \( u \) are genuine almost everywhere) except along curves in the \((x, t)\)-domain \( D \) that have finite-strength solution discontinuities. As hyperbolic conservation laws are usually the limiting case of viscous or viscous-like equations, the piecewise continuous weak solutions satisfy Eq. (2.1) in the sense of distribution theory by satisfying the integral condition
\[
\int_0^\infty \int_{-\infty}^{\infty} \left( u \frac{\partial \varphi}{\partial t} + f \frac{\partial \varphi}{\partial x} \right) dx \, dt + \int_{-\infty}^{\infty} u_0 \varphi_0 \, dx = 0, \tag{2.2}
\]
for any smooth continuously differentiable \( C^\infty \) test function \( \varphi(x, t) \), that vanishes for \(|x|\) and \(t\) large.

Another related integral condition for \( u \) may also be obtained that applies for an arbitrary closed contour \( \delta D' \) containing a portion of the solution domain \( D' \) and can be expressed as [Godunov, 1959]
\[
\oint_{\delta D'} (u \, dx - f \, dt) = 0. \tag{2.3}
\]
As \( u \) does not have to be differentiable everywhere for the integral conditions of Eqs. (2.2) and (2.3) to apply, the equations can be said to be more general statements of the problem than the one given by Eq. 2.1. The equations also furnish the necessary jump conditions for the solution changes at discontinuities. From the integral expression of Eq. (2.2) it can be shown that the well-known Rankine-Hugoniot jump conditions
\[
[f] = s[u], \tag{2.4}
\]
apply across solution discontinuities, where \( s = dx/dt \) is the propagation velocity of the discontinuity and \([f]\) and \([u]\) are the flux and solution jumps across it.

Note that by definition a genuine solution is a generalized solution. Note also that for a given initial condition, there may be more than one generalized solution to the IVP of Eq. 2.1 as weak solutions defined by the integral condition of Eq. (2.2) are not necessarily unique. Usually only one solution is realistic and the ambiguities are resolved by using additional physical information (i.e., so-called entropy conditions) to select the physically correct generalized solution.

It was remarked above that hyperbolic PDEs adequately describe many physical phe-

\(^1\)For problems in gas dynamics, the jump discontinuities are contact surfaces, slipstreams, and shock waves.
nomena. Hence, there is considerable interest in obtaining their solutions. Computational methods are attractive for solving a wide range of problems. However, as the remainder of this chapter will attempt to demonstrate, the occurrence of discontinuities in the generalized solutions of hyperbolic conservation laws, such as those given by Eq. 2.1, can present several numerical challenges.

2.3 Shock-Capturing Methods Versus Shock-Fitting and Shock-Tracking Techniques

Computational schemes for the numerical solution of hyperbolic conservation laws, such as those given by Eq. 2.1, can be classified by type into two distinct categories or groupings [Anderson et al., 1984; Moretti, 1987]. One group of algorithms can be broadly labeled as shock-capturing methods. A second grouping can be identified and referred to as shock-fitting or shock-tracking methods. In shock-fitting or tracking methods, conventional integration techniques appropriate for smooth solutions (e.g., method of characteristics or standard finite-difference methods) are used to solve the governing PDEs in regions where the piecewise continuous weak solutions are genuine and any discontinuities present in the solution are treated in a separate but coupled manner by utilizing the Rankine-Hugoniot jump conditions that result from the integral expressions defining the weak solution, e.g., Eq. (2.4).

On the other hand, in shock-capturing methods, the complete generalized solutions are computed by solving the governing PDEs in conservation (divergence) form without any special treatment of the discontinuities (i.e., shocks are handled automatically and routinely by the solution algorithm). Note that it is possible to make a distinction between shock-fitting and shock-tracking methods. The tag 'shock fitting' is generally more applicable to methods developed for time-invariant problems of hyperbolic conservation laws that fit stationary solution discontinuities [Moretti and Abbett, 1966], whereas, the term 'shock tracking' is more appropriate for methods that track moving solution discontinuities of time-dependent problems [Glimm et al., 1985]. However, the terms are used interchangeably here.

Shock-capturing and shock-fitting methods have their own respective advantages and disadvantages. In shock-fitting methods, discontinuities and shocks are treated as true discontinuities and their solution jump conditions are satisfied exactly. Consequently, generalized solutions may be resolved on relatively coarse numerical grids (i.e., relatively small numbers of points are required in the discretized solution domains). For simple one-dimensional problems and multi-dimensional problems with relatively few discontinuities, shock fitting can be, and has been, performed successfully and efficiently. However, as the nonstationary nature, complexity, and number of discontinuities for the problems increase, the overhead and book-keeping associated with these techniques grow considerably and the methods can become unwieldy. Moreover, some fore-knowledge of the solution is crucial for shock fitting and, therefore, difficulties may also be encountered in correctly identifying and classifying the discontinuities and shock structure for problems with complex nonlinear wave interactions [Glimm et al., 1985].

In contrast to shock-fitting procedures, shock-capturing methods automatically predict the discontinuities of weak solutions and no additional overhead or special procedures are required. The same numerical method can be applied identically in all regions of the solution domain. However, as these methods generally approximate discontinuities by smooth although hopefully steep transitions, a deleterious feature of shock-capturing schemes is that rather refined numerical grids with high node concentrations are often needed to accurately
resolve generalized solutions, particularly for complicated multi-dimensional problems with interacting and/or coalescing shock structure. This is especially true for first-order accurate shock-capturing methods (see Section 2.4.1 below).

Before the mathematical theory of hyperbolic conservation laws had fully matured and sophisticated shock-capturing techniques had evolved, shock-fitting methods were probably the more popular of the two approaches for handling gas-dynamic flows with shocks. The fitting of a boundary shock was, and is still, often used in many steady-flow problems, particularly for supersonic and hypersonic blunt-body flows [Moretti and Abbett, 1966; Moretti, 1987]. Indeed, many of the early solution techniques for gaseous flows with shocks undergoing finite-rate thermochemical nonequilibrium processes were shock-fitting methods (e.g., [Blottner, 1969; Evans et al., 1970]). In addition, shock-tracking has been successfully implemented for predicting the complex two-dimensional time-dependent inviscid flows associated with oblique shock-wave reflections [Glimm et al., 1985]. However, the greater flexibility and often conceptual simplicity offered by shock-capturing techniques, coupled with significant improvements in solution algorithms and computer performance, have resulted in these methods becoming more popular than shock-fitting and shock-tracking techniques. The early attempts at shock capturing are reviewed in the next section.

2.4 Classical Shock-Capturing Methods

2.4.1 Early Finite-Difference Methods

The first pioneering work on shock-capturing techniques for hyperbolic conservation laws was conducted during the 1950s and early 1960s and most of the schemes considered were finite-difference based. Convergence of the methods was a primary concern of early researchers. Very basic questions were asked such as “How can one use a finite-difference solution procedure that apparently requires the existence of continuous derivatives to obtain solutions to hyperbolic conservation laws which admit weak solutions with discontinuities?”. For continuous solutions of PDEs, it was known that the convergence of a finite-difference scheme could be inferred from the consistency and stability of the method, i.e., a consistent stable scheme converges [Anderson et al., 1984; Hirsch, 1989]. In general, a difference scheme is deemed to be consistent if the truncation error, defined to be the difference between the PDEs and the difference representation thereof, tends to zero as the discretized solution domain is refined. Having established consistency, convergence is usually inferred from linear stability by using von Neumann Fourier analysis applied to the linearized equations [Anderson et al., 1984; Hirsch, 1989]. However, there were some doubts as to whether these results were applicable for weak solutions without special treatment of the discontinuities.

One of the first shock-capturing schemes was the q-method proposed by von Neumann and Richtmyer [1950]. In their method, nonlinear artificial dissipation in the form of a viscous-like term $q$ was explicitly added to the conservation equations in such a way that the solutions of the modified PDEs became genuine and the discontinuities of the original equations were replaced by smooth transitions. Care was taken to ensure that the thickness of the smooth shock transitions was always of the order of the mesh spacing and that the effects of the dissipation were negligible away from the transitions. Although discontinuities are not sharply resolved by this scheme and transition zones are smeared over several mesh points, the method was important for it clearly demonstrated the plausibility of shock-capturing techniques.

Following this approach by von Neumann and Richtmyer, Lax [1954] proposed a shock-
capturing scheme for hyperbolic conservation laws that did not require the explicit addition of artificial dissipation. Lax’s method is first-order accurate with the leading term in the truncation error corresponding to the second derivative of the solution and thus, the method is sufficiently dissipative to smooth discontinuities [Anderson et al., 1984]. One significant result of this early work of Lax was that it was demonstrated that a difference method is guaranteed to converge to a weak solution (i.e., shocks represented by smooth transitions propagate with the correct velocity) if the difference scheme is consistent with the conservation form of the PDEs and it converges. What is meant by ‘consistent with the conservation form of the PDEs’? This can be understood by considering the hyperbolic conservation laws of Eq. (2.1). For a uniform discretized spatial domain \( x_i = i\Delta x \) and \( u(i\Delta x, t) = u_i \), where \( \Delta x \) is the node point spacing and \( i \in [0, 1, \ldots, I] \), a \((2k+1)\)-point semi-discrete finite-difference scheme with an appropriate choice of time differencing is said to be consistent with the conservation laws if the solution change \( \partial u/\partial t \) can be written in the form [Lax, 1954; Lax and Wendroff, 1960; Harten, 1983; Harten, 1984]

\[
\left( \frac{\partial u}{\partial t} \right)_i = \frac{-1}{\Delta x} \left( h_{i+1/2} - h_{i-1/2} \right), \tag{2.5}
\]

where \( h_{i+1/2} \) is a numerical approximation to the flux at the interface between nodes \( i \) and \( i+1 \) having the form

\[
h_{i+1/2} = h(u_{i-k+1}, \ldots, u_{i+k}), \tag{2.6}
\]

that is consistent with the flux function \( f(u) \) such that for \( u_{i-k+1} = \cdots = u_{i+k} = u \)

\[
h(u, \ldots, u) = f(u). \tag{2.7}
\]

Here, the integer value \( k \) defines the spatial bandwidth of the method. Note that one direct consequence of this type of construction for the spatial differencing is that only the boundary fluxes at interfaces \( i = 1/2 \) and \( i = I - 1/2 \) contribute to the sum of the flux differences \( h_{i+1/2} - h_{i-1/2} \), i.e.,

\[
-\Delta x \sum_{i=0}^{I-1} \left( \frac{\partial u}{\partial t} \right)_i = \sum_{i=0}^{I-1} \left( h_{i+1/2} - h_{i-1/2} \right) = h_{I-1/2} - h_{1/2}. \tag{2.8}
\]

Hence, methods that are consistent with the convergence form of the PDEs also satisfy a discrete form of the conservation property defined by the integral condition of Eq. (2.3). This is obviously desirable. Schemes of the form of Eq. (2.5) are sometimes termed conservative discretizations [Roe, 1986a].

Another early shock-capturing technique was proposed by Godunov [1959]. This remarkable and original method can be viewed as the first successful conservative upwind scheme as well as the first flux-difference splitting method [Hirsch, 1990]. Like Lax’s method, Godunov’s solution technique also employs a conservative discretization procedure that is consistent with the divergence form of the conservation laws. However, rather than developing formulas for the interface flux from finite-difference approximations, the method makes use of the exact solution of a local Riemann IVP posed between adjacent nodes \( i \) and \( i+1 \) to evaluate the interface numerical flux function \( h_{i+1/2} \). The use of the information from the Riemann problem solution provides Godunov’s scheme with the ability to recog-
nize and correctly propagate shocks and other discontinuities as well as makes certain that the method converges to a physically correct generalized solution. Riemann problems and their solution are discussed in Appendix A. Note that the use of the Riemann problem to resolve discontinuities in a shock-capturing method can, in some ways, be regarded as a clever utilization of shock-tracking concepts.

Although not a finite-difference based scheme, an algorithm that is somewhat related to Godunov's method is the random-choice method (RCM) of Glimm [Glimm, 1965; Gottlieb, 1988]. The RCM, which arose from a theoretical existence proof, is a rather unconventional explicit time-marching shock-capturing method for solving systems of hyperbolic equations. Like Godunov's method, it also makes use of the Riemann problem but instead of using a difference formulation to update the solution, the values of the approximate RCM solution at new time levels are obtained by sampling the exact Riemann problem solutions at randomly chosen points within each grid interval. A random number sequence is used to direct the solution sampling and so, in a sense, the RCM may be regarded as a Monte Carlo technique. The important advantages of the method are the sharp resolution of discontinuities and the absence of the usual dissipative and dispersive truncation errors associated with finite-difference and finite-volume methods. In one space dimension, considerable success has been achieved [Gottlieb, 1988; Groth and Gottlieb, 1988; Zhang and Gottlieb, 1986]. Unfortunately, useful extensions of the RCM to more than one spatial dimension have not been forthcoming.

In summary, these first attempts at shock capturing were in fact quite successful. The shock-capturing concept appeared to be justified and the use of a conservative discretization procedure and the Riemann problem were shown to be helpful in ensuring good numerical results. Nevertheless, most of the early finite-difference methods were explicit, three-point, first-order accurate time-marching schemes. Whether by the explicit addition of artificial viscosity or through the inherent (implicit) dissipation introduced by the differencing formulation, almost all of these schemes, with the exception of the RCM, were heavily dissipative with strong smearing of discontinuities (see the example calculation of Figure 2.1 and notice particularly the smearing of the contact surface). Therefore, unless excessively refined computational meshes were used, it was generally felt that the solution quality of these first-order methods near shocks was unsatisfactory for many applications, especially nonstationary multi-dimensional problems of gas dynamics. This led to a search for more accurate solution methods.

Before continuing, it should be pointed out that much of the early research into shock-capturing techniques was aided, to a large extent, by the development of the mathematical theory of hyperbolic systems of conservation laws, which matured greatly during the time period. Mathematicians have considerable interest in numerical techniques for they offer the possibility of proving the existence of solutions to IVPs with arbitrary initial data.

### 2.4.2 Higher-Order Finite-Difference Methods

In an effort to improve the accuracy and reduce the grid-point requirements of shock-capturing methods, both explicit and implicit second-order accurate finite-difference representations of hyperbolic conservation laws were investigated during the 1960s and early 1970s. A number of second-order shock-capturing schemes were devised. These included the second-order explicit method of Lax and Wendroff [1960], the explicit predictor-corrector scheme of MacCormack [MacCormack, 1969; MacCormack and Paullay, 1972], the explicit second-order upwind scheme of Warming and Beam [1976], and the implicit centered-
difference method of Beam and Warming [1976]. In some cases, even greater accuracy was sought by considering third-order methods [Rusanov, 1970].

Compared with the early first-order methods, all of the above spatially second-order accurate schemes have greater solution accuracy and reduced numerical dissipation. Hence, the predicted transitions at shocks and discontinuities are noticeably thinner than those of first-order methods for the same mesh spacing. Unfortunately, although affording some measure of improvement in shock resolution, these first attempts at achieving greater accuracy have deficiencies. The major drawback of the second-order schemes is that the discrete solutions contain spurious Gibb's-like oscillations. Post-shock oscillations can be observed for centered difference methods and pre-shock oscillations can be found in the solutions of the second-order upwind schemes (both pre- and post-shock oscillations can be observed in the solutions of third-order methods). The numerical results depicted in Figure 2.2 are illustrative of these types of solution errors. (The results of the method evaluation study by Emery [1968] are also indicative of the difficulties.) The overshoots and undershoots in these higher-order approximations can be shown to be due to numerical dispersion [Anderson et al., 1984; Hirsch, 1990]. The lowest-order truncation error for most second-order methods is a dispersive one and, for high-frequency or short wavelength solution content (i.e., near shocks), these leading and/or lagging phase errors can become large.

For many applications, such as the solution of high-speed nonequilibrium flow problems that are of interest here, the Gibb's-like phenomena associated with the preceding second-order methods can be very detrimental. For example, solution undershoots can readily lead to the occurrence of a negative value in the computed flow density or an aphysical value for the calculated flow internal energy. In addition, the oscillations can create several difficulties when attempting to predict species concentrations for reactive flow problems.

### 2.4.3 Artificial Dissipation

The solution quality of the classical second-order shock-capturing methods was generally considered to be inadequate and various means by which the dispersive oscillations could be suppressed were explored. It was recognized that the numerical instabilities in the vicinity of shocks could be controlled and even eliminated by adding artificial dissipative (viscous-like) terms to the difference equations. The addition of dissipative terms has the effect of actually modifying the form of the original difference scheme. Removal of the dispersive oscillations is accomplished by reducing the accuracy of the unmodified higher-order method where solution gradients are large towards that of a first-order scheme which does not exhibit the oscillations. Although rather simple in principle, there were difficulties in the implementation of these so-called artificial-viscosity methods. Most of the problems related to the choice of dissipation.

In general, the magnitude of the dissipation required to alleviate dispersive oscillations near discontinuities was found to be quite problem dependent. Moreover, the added dissipation was observed to have two unwanted effects: 1) it tended to thicken shocks; and 2) it unnecessarily deteriorated the solution quality in smooth continuous regions. Thus, in selecting the amount of artificial viscosity, a careful balance was needed between the desire for oscillation-free solutions near discontinuities and the desire for greater accuracy in smooth regions. Solution-dependent artificial viscosity was evidently appropriate; however, the form it should take was neither obvious nor clear. One obstacle at the time was that a theoretical foundation for the selection of the dissipation terms was unavailable. The well-established linear theory could only serve as a rough but unreliable guide in early attempts.
to design optimal artificial-viscosity techniques. Much empiricism and imprecision existed and, in many schemes, considerable tuning of the coefficients controlling the addition of artificial dissipation was required to obtain reasonable solutions with minimal oscillations. Although sophisticated artificial-viscosity methods have been developed and are still used in many applications today (see, for example, Harten and Zwas [1972], Pulliam [1986], and Hirsch [1990]), these methods are generally considered to be non-optimal because they lack a certain robustness and cannot provide the best solutions for problems involving strong discontinuities, complex nonlinear wave interactions, and/or highly transient phenomena.

2.4.4 Preservation of Solution Monotonicity

The difficulties associated with the application of classical finite-difference techniques for the computation of weak solutions to hyperbolic PDEs can be summarized as follows. Given monotonic initial data (i.e., initial distributions with constantly increasing or decreasing solution profiles) for which the unique weak solution remains monotonic at later times (this is the case for single solution discontinuity), the approximate solutions of high-order schemes do not always remain monotonic. New local minima (undershoots) and maxima (overshoots) in the computed solutions form and give rise to persistent dispersive oscillations near shocks. On the other hand, the solutions of first-order schemes appear to remain monotonic. Regrettably, first-order accuracy is insufficient for most practical purposes. Although some success can be achieved by employing a higher-order technique and adding artificial dissipation to damp oscillations around discontinuities, for these schemes, either excessive damping is used or oscillations are unavoidable for all problems. These statements more or less represent the status of shock-capturing techniques in the early 1970s.

Further insight into these difficulties may be gained by considering the linear scalar version of the conservation laws given by Eq. (2.1) for which $f = au$, where $a$ is a constant, and by applying a consistent $(2k+1)$-point explicit one-step time-stepping finite-difference scheme of the form expressed by Eq. (2.5) to this linear PDE. Letting $u(iΔx, nΔt) = u^n_i$ and $t^n = nΔt$ where $Δt$ is the time step, the solution scheme can be expressed as

$$u^n_{i+1} = u^n_i - \frac{aΔt}{Δx} \left( \tilde{u}^{n}_{i+1/2} - \tilde{u}^{n}_{i-1/2} \right), \quad (2.9)$$

where

$$\tilde{u}^{n}_{i+1/2} = \tilde{u}(u^n_{i-k+1}, \ldots, u^n_{i+k}). \quad (2.10)$$

It is easy to show that all linear constant-coefficient finite-difference approximations of the form given by Eqs. (2.9) and (2.10) can be rewritten alternatively as

$$u^n_{i+1} = \sum_{m=-k}^{k} C_m u^n_{i+m}, \quad (2.11)$$

where $C_m$ are the constant coefficients defining the scheme.

In order to examine the discrete solutions of Eq. (2.11), the monotonicity preserving properties of the scheme are defined as follows. After Harten [1983], a solution method for the scalar hyperbolic conservation laws of Eq. (2.1) is said to be monotonicity preserving if with increasing time $t$: 1) no new local solution extrema in $x$ are created; 2) the value of a
local solution minimum is nondecreasing; and 3) the value of a local solution maximum is nonincreasing. It can then be shown that the linear finite-difference scheme of Eq. (2.11) is monotonicity preserving if and only if

$$C_m \geq 0,$$

for $$-k \leq m \leq k$$ from which it follows that the monotonicity preserving forms of Eq. (2.11) are at most first-order accurate [Godunov, 1959; Harten, 1983]. This means that, at least for the linear scalar of PDE of Eq. (2.1), there are no linear constant-coefficient second-order methods having the form of Eq. (2.11) that are monotonicity preserving and non-monotonic solution profiles must occur when linear second-order schemes are used. This rather profound result was first demonstrated by Godunov [1959]. He also argued that a similar conclusion can be drawn for implicit linear difference schemes.

At first glance, the preceding results appear to present a dilemma. Simplistically, it would seem that: 1) all aspirations of higher accuracy are negated by the monotonicity preserving constraints; and 2) a low-order scheme with poor resolution is required for oscillation-free solutions. Additional support for these statements is offered by the non-monotonic oscillatory nature of the second-order finite-difference based shock-capturing techniques discussed so far which, with the exception of the more sophisticated artificial-viscosity techniques mentioned above, can all be shown to be linear when applied to a one-dimensional linear scalar hyperbolic PDE. The key notion in resolving this apparent dilemma is however the linear aspect of the schemes and constraints. The previous statements concerning solution monotonicity do not preclude nonlinear, hybrid, or solution-dependent schemes (e.g., the coefficients $$C_m$$ are not constants but are rather functions of the solution) that are both monotonicity preserving and higher-order accurate. Thus, rather than presenting a dilemma, Godunov’s monotonicity constraints actually offer a means for probable success: higher-order accurate schemes must be highly nonlinear, even for the case of linear PDEs, if monotonicity preserving solutions are to be attained. Note that artificial-viscosity methods attempt to side-step Godunov’s monotonicity constraints by employing dissipative terms that are nonlinearly dependent on the local discrete solution.

Guided by the experience gained from studies with second-order artificial-viscosity methods as well as the constraints imposed by monotonicity considerations (i.e., that linear stability analysis cannot provide the necessary answers for monotonicity preserving solutions and nonlinearity of the solution method is essential), research on the design of more favourable shock-capturing techniques continued during the 1970s and 1980s. Nonlinear solution-dependent schemes that possessed monotonic solution properties and higher-order accuracy were sought. This research eventually led to the modern shock-capturing methods.

### 2.5 Modern Shock-Capturing Methods

The recognition that classical first-order shock-capturing schemes require excessive grid refinement to resolve the complicated shock structure and second-order schemes lead to spurious Gibb's-like oscillations or nonlinear instabilities near discontinuities, spurred continued research into shock-capturing techniques for hyperbolic conservation laws. In the last 10–15 years, innovative advances have led to the development of several high-resolution nonlinear monotonicity preserving schemes. The first among these methods were the flux-corrected transport (FCT) method of Boris and Book [Boris and Book, 1973; Zalesak,
The FCT method of Boris and Book was a two-stage method consisting of a transport (diffusive) first stage followed by a second solution enhancing antidiffusion stage which by design, as Boris and Book state, "should generate no new maxima or minima in the solution, nor should it accentuate already existing extrema". The scheme proposed by van Leer was a nonlinear weighting of the Lax-Wendroff central and Warming-Beam upwind differencing schemes. In both cases, some form of limiting function or limiter was used to control oscillations. Following the success of these schemes, other subsequent methods were devised. Some examples of these techniques are the various higher-order Godunov-type methods such as the monotonic upstream-centered scheme for conservation laws (MUSCL) of van Leer [1979], piecewise parabolic method (PPM) of Colella and Woodward [1984], generalized Riemann problem (GRP) method of Ben-Artzi and Falcovitz [1984], and weighted-average-flux (WAF) method of Toro [1989], as well as the upwind and symmetric TVD schemes of Harten [1983; 1984], Roe [Roe, 1981; Roe and Pike, 1984; Roe, 1984], Davis [1984], Yee [1987a; 1987b], and Osher and Chakravarthy [Osher and Chakravarthy, 1984; Chakravarthy and Osher, 1985a; Chakravarthy and Osher, 1985b]. More recently, the essentially non-oscillatory (ENO) schemes of Harten et al. [1987] have been proposed. All of these nonlinear explicit and/or implicit time-stepping methods provide monotonic oscillation-free solutions and increased accuracy near discontinuities. See Figure 2.3 and compare with Figures 2.1 and 2.2.

The TVD concepts of Harten [1983; 1984] have proven to be useful criteria in developing some of the more popular modern shock-capturing methods. Although many of the schemes mentioned above, such as the FCT method and some of the Godunov-type schemes, were not derived by making explicit use of TVD theory, almost all of these techniques can be shown to be TVD, at least in the case of a scalar conservation law. Before going on to discuss the application of modern shock-capturing schemes to problems in nonequilibrium gas dynamics, TVD theory is first reviewed.

2.5.1 Total-Variation-Diminishing Schemes

It was noted by Harten [1983; 1984] that the usual practice of inferring convergence of numerical solutions by demonstrating the consistency and linear stability of the method did not appear to yield fully satisfactory schemes for the accurate numerical solution of hyperbolic conservation laws. In an attempt to design higher-order monotonic (monotonicity preserving) finite-difference based methods for hyperbolic PDEs without the uncertainty in performance that was found with schemes designed using linear von Neumann stability theory coupled with artificial viscosity techniques, Harten developed a new convergence theorem using the concept of total variation. Armed with this theorem, he was then able to devise effective higher-order nonlinear finite-difference schemes.

In the following sections, the basic principles and concepts of TVD finite-difference schemes are reviewed. The presentation of TVD theory herein does not so much describe details of TVD methods but, rather, provides an overview of the tools and methodology for designing such schemes. Detailed descriptions of specific methods can be found elsewhere.

---

2One notable exception are ENO schemes. ENO schemes are not guaranteed to be TVD and form a larger class of schemes that encompasses those that are TVD [Harten et al., 1987].
Linear and Nonlinear Scalar Hyperbolic Conservation Laws in One Dimension

Consider first the scalar version of the one-dimensional hyperbolic PDEs represented by Eq. (2.1). For this restricted case, it follows from Harten that the total variation of a discrete numerical solution \( u_i^n \) in the spatial coordinate \( x \) is defined as

\[
TV(u^n) = \sum_i \left| \Delta u_{i+1/2}^n \right| = \sum_i \left| u_{i+1}^n - u_i^n \right| ,
\]

(2.13)

for a uniform discretized solution domain \( x_i = i \Delta x, t^n = n \Delta t \) with \( u(i \Delta x, n \Delta t) = u_i^n \), where \( \Delta x \) is the node point spacing, \( \Delta t \) is the time step, and \( i \in [-\infty, \ldots, -1, 0, 1, \ldots, \infty] \) and \( n \in [0, 1, \ldots, N] \). From this, the notions of total-variation stable and TVD (total-variation diminishing) can be defined. A numerical solution is deemed to be of bounded total variation or total-variation stable if there exists a constant \( C \) such that

\[
TV(u^n) \leq C TV(u^0) ,
\]

(2.14)

and a discrete solution is said to be TVD if

\[
TV(u^{n+1}) \leq TV(u^n) .
\]

(2.15)

If the definition of Section 2.4.4 is then used to identify monotonicity preserving approximate solutions of Eq. (2.1), then the following theorem has been proven by Harten [1983].

**Theorem 2.1 (Harten) A TVD scheme is monotonicity preserving.**

Having established these concepts, the convergence theorem of Harten [1984] can be stated.

**Theorem 2.2 (Harten) If a numerical scheme is both consistent with the conservation law of Eq. (2.1) in the sense of Eqs. (2.5)-(2.7) and the appropriate entropy condition, and if the resulting numerical approximation is total-variation stable, then the scheme is convergent and its limit is the unique weak solution of Eq. (2.1) that satisfies the appropriate entropy condition.**

Refer to the original work for proof of this theorem and a definition of the entropy condition that is satisfied. Note that total-variation stable is a weaker condition than TVD and thus, the convergence theorem applies equally well to TVD schemes.

Conditions for both 3- and 5-point explicit and implicit schemes to be TVD have been derived by Harten [1983; 1984]. The main results for the more significant 5-point schemes can be summarized as follows. Consider 5-point schemes of the form

\[
u_i^{n+1} + \Theta \frac{\Delta t}{\Delta x} \left( h_{i+1/2}^{n+1} - h_{i-1/2}^{n+1} \right) = u_i^n - (1 - \Theta) \frac{\Delta t}{\Delta x} \left( h_{i+1/2}^n - h_{i-1/2}^n \right) ,
\]

(2.16)

with consistent numerical flux functions

\[
h_{i+1/2}^n = h(u_{i-1}^n, u_i^n, u_{i+1}^n, u_{i+2}^n), \quad h_{i-1/2}^n = h(u_{i-2}^n, u_{i-1}^n, u_i^n, u_{i+1}^n),
\]

(2.17)

and where \( \Theta \) is a time-stepping control parameter. The scheme is: 1) Euler explicit for
\( \Theta = 0 \); 2) trapezoidal implicit for \( \Theta = 1/2 \); and 3) Euler implicit for \( \Theta = 1 \). The difference method of Eq. (2.16) can be re-expressed as

\[
\begin{align*}
    u_{i+1}^{n+1} + \lambda \Theta \left[ C_{i+1/2}^{n+1} \Delta u_{i+1/2}^{n+1} - C_{i-1/2}^{n+1} \Delta u_{i-1/2}^{n+1} \right] = \\
    u_i^n + \lambda (1 - \Theta) \left[ C_{i+1/2}^{n} \Delta u_{i+1/2}^{n} - C_{i-1/2}^{n} \Delta u_{i-1/2}^{n} \right],
\end{align*}
\]  

(2.18)

for which

\[
C_{i+1/2}^{n} = C^{-}\left( u_{i-1}^{n}, u_{i}^{n}, u_{i+1}^{n}, u_{i+2}^{n} \right), \quad C_{i-1/2}^{n} = C^{+}\left( u_{i-2}^{n}, u_{i-1}^{n}, u_{i}^{n}, u_{i+1}^{n} \right),
\]

(2.19)

and where \( \Delta u_{i+1/2}^{n} = u_{i+1}^{n} - u_{i}^{n} \) and \( \lambda = \Delta t/\Delta x \). Note that the general form of \( C^{+} \) and \( C^{-} \) clearly illustrate the nonlinearity of the schemes. It can then be proven that the sufficient conditions ensuring that the scheme of Eq. (2.18) is TVD are as follows:

\[
\begin{align*}
    \lambda (1 - \Theta) C_{i+1/2}^{n+} &\geq 0, \quad \lambda (1 - \Theta) C_{i+1/2}^{n-} \geq 0, \\
    \lambda (1 - \Theta) \left( C_{i+1/2}^{n+} + C_{i+1/2}^{n-} \right) &\leq 1, \\
    -\lambda \Theta C_{i+1/2}^{n+} &\leq 0, \quad -\lambda \Theta C_{i+1/2}^{n-} \leq 0,
\end{align*}
\]

(2.20) (2.21) (2.22)

for all values of \( n \) and \( i \).

The five point finite-difference scheme of Eq. (2.16) is consistent with the scalar PDE and if the conditions of Eqs. (2.20)-(2.22) are met, the scheme is also TVD. Thus, in order to prove convergence to the unique weak solution in terms of Theorem 2.2, all that remains to be established is that the scheme is consistent with the appropriate entropy condition. Harten was unable to prove rigorously that the TVD schemes are consistent with the entropy condition. Although such a proof is unavailable, it has been shown that: 1) in the linear scalar case ( \( f = au \), where \( a \) is a constant), the 5-point TVD schemes are convergent to the unique weak solution; 2) all first-order explicit forward Euler 5-point TVD schemes (\( \Theta = 0 \)) are also convergent to the unique weak solution; 3) all second-order 5-point TVD schemes are convergent to a weak solution; and 4) numerical experiments indicate that the TVD schemes are consistent with the entropy condition.

Equations (2.16)-(2.22) coupled with Theorems 2.1 and 2.2 represent a powerful set of tools for designing nonlinear higher-order shock-capturing methods for linear and nonlinear scalar hyperbolic conservation laws that afford sharp resolution of discontinuities and are monotonicity preserving (i.e., oscillation free). It is interesting to note that TVD theory now supplies the previously unavailable theoretical basis or non-empirical rationale for constructing artificial dissipation mechanisms which would provide the artificial-viscosity methods discussed earlier in this chapter with high-resolution non-oscillatory solution characteristics [Davis, 1984; Roe, 1984]. The design of a TVD scheme can proceed by selecting a first-order TVD scheme and adding terms that make the method higher-order. Nonlinear limiting functions must be devised to restrict the magnitude of the higher-order terms and ensure that the sufficient conditions of Eqs. (2.20)-(2.22) are satisfied. Alternatively, the design can proceed by starting with the desired high-order \emph{unlimited} difference scheme and then devising nonlinear limiters for the flux functions that make the method TVD. Various techniques are possible and a number of upwind and symmetric TVD schemes have been developed. (See, for example, Harten [1983; 1984], Roe and Pike [1984], Roe [1984], Davis [1984], Osher and Chakravarthy [1984], Sweby [1984], and Yee [1987a; 1987b]. See also the
text of Hirsch [1990].) Obviously, key ingredients in the design of TVD schemes are the nonlinear limiting functions or limiters. Both slope and flux limiters are possible and the appropriate choice depends to a large degree on the discretization procedure adopted. An excellent survey of flux limiters for hyperbolic conservation laws is given by Sweby [1984].

In regard to TVD solution accuracy, the convergence theorem and its proof do not provide error estimates for the finite-difference schemes. The higher-order schemes that satisfy the sufficient conditions for TVD presented above must all reduce to first-order near extrema. However, numerical experiments clearly indicate that even though solution accuracy deteriorates to first-order in some localized regions of the solution domain, the computed higher-order solutions are considerably more accurate than first-order results and hence, the term higher-order is generally taken to mean higher-order almost everywhere.

**Extensions to Hyperbolic Systems and Multidimensions**

Extensions of the scalar TVD schemes described above to the more interesting case of one-dimensional hyperbolic systems of conservation laws, where $u$ and $f$ are now vectors, are usually accomplished by employing some form of flux-vector splitting [Steger and Warming, 1981; van Leer, 1982] or flux-difference splitting [Roe, 1981], the latter requiring the use of either exact or approximate Riemann solvers (see Appendix A). For hyperbolic systems in one space dimension, Harten [1983; 1984] has adopted a variant of the flux-difference splitting procedure of Roe [1981] and has shown that the resulting TVD schemes are convergent to the unique weak solution for linear systems of conservation laws. Note that the associated proof requires the slight redefinition of the total variation of the solution. However, in the case of nonlinear systems, the total variation would no longer appear to precisely define the desired monotonic behaviour of a solution. Unlike the scalar and linear system cases, the solutions of nonlinear systems permit the interaction of nonlinear waves and these interactions can result in the increase in the total variation of the solution. For example, in gas dynamics, the collision of two oppositely propagating shocks will result in an increase in the solution variation. For these reasons, Harten was unable to prove convergence of the proposed flux-difference split TVD schemes for nonlinear systems. Nevertheless, numerical experiments demonstrate that the schemes perform well.

The extension of TVD schemes for the solution of hyperbolic conservation laws in two- or three-space dimensions is normally achieved by utilizing some form of dimension splitting which usually results in a series of one-dimensional solution operators, one for each space dimension. The TVD concepts described above can then be applied to each one-dimensional operator. It is obviously questionable whether multidimensional algorithms developed in this manner are TVD. Furthermore, the accuracy of the multidimensional scheme is also uncertain. Goodman and LeVeque [1985] indicate that time-split TVD algorithms applied to two-dimensional systems are, at most, first-order accurate. However, once again, numerical experiments provide evidence of good results. Note that research on truly multidimensional shock-capturing algorithms is ongoing [Roe, 1986b; Powell et al., 1990].

### 2.5.2 Application of Modern Shock-Capturing Methods to Compressible Thermochemical Nonequilibrium Flows

Most of the TVD and other modern shock-capturing schemes described previously were either developed specifically for, or have subsequently been extended to, the solution of multidimensional flows of polytropic gases (thermally and calorically perfect). In this respect, the
use of Riemann problems and exact Riemann solvers as first advocated by Godunov [1959], the flux-vector splitting techniques of Steger and Warming [1981] and van Leer [1982], and the flux-difference splitting procedure of Roe [1981] and associated approximate Riemann solvers were all helpful. The modern methods offer a reliable means by which to solve complicated compressible flows with complex nonlinear wave interactions involving shock waves, contact surfaces, and slip streams. They are appropriate for steady and unsteady high-speed (hypersonic) flow applications; however, further extensions of the algorithms are necessary for the study of flows with high-temperature and real-gas phenomena.

For high-speed flows in which the density of a gas is relatively large (e.g., flows normally encountered in hypersonic flight at lower altitudes), the mean free paths of the molecules and atoms are such that the molecular collisional rate is high and the assumption of complete thermodynamic equilibrium is a valid approximation. In this case, it is possible to include real-gas effects by describing the thermodynamic state variables of a gas in terms of a single equilibrium temperature (representing the total specific internal energy) and the density. The governing conservation laws remain virtually unchanged from the polytropic case. A number of the aforementioned modern shock-capturing schemes have been extended to include equilibrium high-temperature and real-gas effects (e.g., [Colella and Glaz, 1985; Glaister, 1988a; Glaister, 1988b; Glaister, 1988d; Vinokur and Liu, 1988; Grossman and Walters, 1989; Montagné et al., 1989; Liou et al., 1990; Suresh and Liou, 1991]). Provided that thermodynamic properties are evaluated in an efficient manner, these equilibrium flow solvers are computationally efficient and afford sharp resolution of discontinuities.

For lower density high-speed flows (e.g., flows usually encountered in hypersonic flight at higher altitudes) in which the continuum assumption still applies but the molecular collisional rates are sufficiently low, it is not always possible for a gas to maintain thermodynamic equilibrium. Nonequilibrium effects such as vibrational and chemical rate processes become important. The mathematical modeling of gaseous flows predominated by such finite-rate thermochemical processes necessitates the introduction of additional conservation equations, often containing inhomogeneous source terms, in order to account for the various species and internal energy modes of a nonequilibrium mixture. As a result, extensions of the shock-capturing techniques for nonequilibrium flows require more attention. Discrete numerical solutions satisfying monotonicity as well as positivity and maximum principles are sought for large systems of conservations laws with often large inhomogeneous source terms. In many cases, the large source terms make the solution algorithms stiff (i.e., as in the solution of stiff systems of ordinary differential equations, the time stepping of a marching procedure is drastically constrained by stability considerations rather than by the usual accuracy concerns). This is problematic because the computational requirements for solving large systems with inherent numerical stiffness may become enormous. Furthermore, LeVeque and Yee [1990] as well as Griffiths et al. [1992] have shown that if the source terms are sufficiently stiff then numerical schemes may propagate solution discontinuities, such as shocks, at incorrect or non-physical wave speeds. Thus, shock-capturing schemes for nonequilibrium flows must be designed to provide accurate results in an efficient manner.

Several explicit, semi-implicit, and fully implicit time-stepping MUSCL-type and TVD approaches have been devised for the prediction of nonequilibrium flows. Eberhardt and Brown [1987] extended a first-order explicit TVD upwind scheme for investigating chemically reacting flows. A fourth-order Runge-Kutta time differencing of the source terms was employed to enhance stability and the gas-dynamic and species conservation equations were solved in a fully coupled manner. Glaz et al. [1988] have developed an explicit second-order Godunov (MUSCL-like) method for predicting nonequilibrium vibrationally relaxing
and chemically reacting flows, in which the gas-dynamic and thermodynamic equations are solved in a time-split (decoupled) fashion. Ben-Artzi [1989] also describes a reformulation of the explicit GRP method for chemically reacting flows. Explicit time differencing (second- and fourth-order Runge-Kutta procedures) of the source terms is again used in both of these methods. In other studies, Liu and Vinokur [1989] and Shuen et al. [1990] considered the most general case of nonequilibrium flow and present formulas for the numerical evaluation of inviscid fluxes using several upwind flux-splitting methods.

The explicit time-stepping schemes described above are valid for time-accurate and steady-state calculations of nonequilibrium flows. However, the stiffness of the source terms may force the time step of explicit schemes to be excessively small and the corresponding computer times to be prohibitively large, especially for steady-state computations. Thus, implicit solvers for nonequilibrium flows have also been formulated. In these methods, the numerical stability is enhanced by treating some or all terms implicitly. Yee and Shinn [1989] and Ben-Artzi [1989] propose fully coupled semi-implicit extensions of symmetric TVD and GRP techniques, respectively, for the computation of chemically reacting flows. These schemes treat only the source terms implicitly and therefore avoid large matrix inversions. They are similar to the semi-implicit methods of Bussing and Murman [1988].

Gnoffo and McCandless [1986], Gnoffo et al. [1987], and Gnoffo [1989] have proposed both loosely and fully coupled fully implicit algorithms which use a second-order symmetric TVD scheme of Yee [1987a; 1987b] to solve steady viscous hypersonic flows of air and include the effects of vibrational relaxation, dissociation/recombination, and ionization. Similar fully implicit procedures are discussed by Yee and Shinn [1989] for chemically reacting flows only. Their paper includes discussions of techniques with both implicit and explicit coupling between fluid and species equations. In addition, Molvik and Merkle [1989] and Slomski et al. [1990] describe fully implicit and implicit multigrid solution procedures, respectively, for chemically reacting flows. Both of these algorithms are based on extensions to the TVD upwind schemes of Osher and Chakravarthy [Osher and Chakravarthy, 1984; Chakravarthy and Osher, 1985a; Chakravarthy and Osher, 1985b]. Point relaxation is employed by Gnoffo et al. and Yee and Shinn for the solution of the associated large nonlinear system of equations. This stratagem is computationally efficient because it does not necessitate the direct inversion of large block banded matrices. Molvik and Merkle use approximate factorization in conjunction with a modified Newton iteration technique in their solution procedure, whereas, Slomski et al. employ approximate factorization in conjunction with a multigrid convergence acceleration procedure.

In other recent studies, Park and Yoon [1991] have developed a fully coupled implicit algorithm that uses a flux-limited dissipation model to evaluate the higher-order numerical fluxes and a lower-upper factorization procedure that does not require the inversion of large banded matrices. As well, a comprehensive set of characteristic-based upwind techniques, that use any of three flux splitting procedures (Steger-Warming, van Leer, and Roe) in concert with either explicit Runge-Kutta, implicit approximate-factorization, or implicit lower-upper decomposition time integration schemes, are described by Walters et al. [1992] for computing steady-state solutions of thermochemical nonequilibrium flows. In particular, their results emphasize the fact that explicit Runge-Kutta methods are generally inappropriate for nonequilibrium flow solution, at least for stationary flow applications.

The preceding list of nonequilibrium flow solvers is by no means inclusive. It does, however, provide an indication of some of the more common means by which many of the popular shock-capturing methods have been adapted for solving flows that are in chemical and/or thermal nonequilibrium. It should be noted that a number of the papers given in
the proceedings of the recent IUTAM Symposium on Aerothermochemistry of Spacecraft and Associated Hypersonic Flows [Brun et al., 1992] describe other sophisticated shock-capturing algorithms for thermochemical nonequilibrium flow solution.

2.6 Preview of Proposed Shock-Capturing Methods for Thermochemical Nonequilibrium Flows

In accordance with the goals defined in Chapter 1, this thesis will describe partially-decoupled semi-implicit and factored implicit TVD FDS finite-difference schemes for the solution of the conservation laws governing two-dimensional inviscid nonequilibrium vibrationally relaxing and chemically reacting flows of thermally-perfect gaseous mixtures in a generalized transformed coordinate system. These schemes are variants of some of the techniques discussed above. In both the time-split semi-implicit and factored fully implicit methods, the gas-dynamic and thermodynamic equations are partially decoupled by employing a frozen flow approximation. The two sets of decoupled equations are then solved alternately in a lagged manner within a time marching procedure, thereby providing explicit coupling between the fluid conservation laws and the species concentration and vibrational energy equations. The semi-implicit formulation, based on Roe's higher-order TVD flux-differencing scheme [Roe, 1981; Roe and Pike, 1984], is more appropriate for unsteady applications. The factored implicit form, based on Chakravarthy and Osher's high-resolution TVD schemes [Osher and Chakravarthy, 1984; Chakravarthy and Osher, 1985a; Chakravarthy and Osher, 1985b], is useful for obtaining steady state solutions. An extension of Roe's approximate Riemann solver [Roe, 1981; Glaister, 1988d], giving the eigenvalues and eigenvectors of the fully coupled system, is used in the flux-difference splitting procedures for evaluating the numerical flux functions of both algorithms. Various modifications to the Riemann solutions are also described which ensure that physically realistic solutions are obtained. The proposed partially-decoupled methods are shown to have several advantages over other chemistry-split and fully coupled techniques. Chapter 3 gives a description of the two-dimensional conservation laws that are of interest here and the TVD schemes are then presented in Chapter 4. The numerical predictions of Chapter 6, using a five-species four-temperature thermodynamic model for air (see Appendix C), illustrate the capabilities of the techniques.

As well, a multigrid version of the fully implicit upwind TVD scheme is proposed for the more efficient computation of steady time-invariant solutions of the governing two-dimensional nonequilibrium flow conservation laws. The multigrid algorithm is based on the full approximation storage (FAS) and full multigrid (FMG) concepts and employs the partially-decoupled factored implicit FDS TVD scheme as the smoothing operator in conjunction with a four-level V-cycle coarse-grid-correction (CGC) procedure. A combination simple-injection/full-weighted restriction operator and a bilinear interpolation prolongation operator are used. The implicit multigrid technique is outlined in Chapter 5 and a few numerical examples demonstrating the effectiveness of method are presented in Chapter 7.
Figure 2.1: One-dimensional Euler equation solution $u = [\rho, \rho u, p/(\gamma - 1) + \rho u^2/2]^T$ to unsteady shock-tube problem (air, $\gamma = 1.4$, $\rho_l = 4.69 \text{ kg/m}^3$, $u_l = 0 \text{ m/s}$, $u_r = 0 \text{ m/s}$, $p_l = 101.1 \text{ kPa}$, $\rho_r = 1.41 \text{ kg/m}^3$, $u_r = 0 \text{ m/s}$, $p_r = 404.4 \text{ kPa}$). Numerical results for first-order method of Godunov (100 node points).
Figure 2.2: One-dimensional Euler equation solution \( \mathbf{u} = [\rho, \rho u, p/(\gamma - 1) + \rho u^2/2]^T \) to unsteady shock-tube problem (air, \( \gamma = 1.4, \rho_l = 4.69 \text{ kg/m}^3, u_l = 0 \text{ m/s}, u_l = 0 \text{ m/s}, p_l = 101.1 \text{ kPa}, \rho_r = 1.41 \text{ kg/m}^3, u_r = 0 \text{ m/s}, p_r = 404.4 \text{ kPa}). Numerical results for second-order predictor-corrector method of MacCormack (100 node points).
Figure 2.3: One-dimensional Euler equation solution \( \mathbf{u} = [\rho, \rho u, \rho u^2/(\gamma - 1) + \rho u^2/2] \) to unsteady shock-tube problem (air, \( \gamma = 1.4 \), \( \rho_l = 4.69 \text{ kg/m}^3 \), \( u_l = 0 \text{ m/s} \), \( u_t = 0 \text{ m/s} \), \( p_l = 101.1 \text{ kPa} \), \( \rho_r = 1.41 \text{ kg/m}^3 \), \( u_r = 0 \text{ m/s} \), \( p_r = 404.4 \text{ kPa} \)). Numerical results for higher-order upwind TVD scheme of Roe (100 node points).
Chapter 3

Conservation Laws of Inviscid Compressible Gaseous Flows: The Euler Equations

3.1 Introductory Remarks

This chapter of the dissertation provides a description of the conservation equations of mass, momentum, and energy for inviscid (non-heat-conducting) compressible thermochemical nonequilibrium and equilibrium continuum gaseous flows. These PDEs, generally referred to as the Euler equations, are the limiting form of the more general conservation equations for viscous flow (the Navier-Stokes equations) as the flow Reynolds number approaches infinity. The discussion will include a development of the equations for a general Cartesian coordinate system as well as for two-dimensional planar generalized curvilinear coordinates, the latter being the case of primary interest to the present numerical study.

As noted in the introductory chapters, the efficient numerical solution of the Euler equations for flows in which the gas is in both thermal and chemical nonequilibrium is the focus here and, in the next chapter, TVD flux-difference split methods are proposed for the numerical solution of the conservation equations in this case. However, in Chapters 6 and 7, numerical results for the case of thermal and chemical equilibrium are also considered. This is done for comparison purposes when evaluating the predictive capabilities of the proposed nonequilibrium flow solution techniques. Thus, for the sake of completeness, the Euler equations governing both nonequilibrium and equilibrium flows are given in this chapter.

3.2 Thermal and Chemical Nonequilibrium Flows

3.2.1 Physical Assumptions

For the thermochemical nonequilibrium analysis described herein, it is assumed that the dynamic behaviour of the gaseous fluid of interest can be accurately represented by an inviscid continuum. The continuum assumption is certainly true for most gas dynamic flows with Knudsen numbers, Kn, less than 0.02 [Anderson, 1989]. The Knudsen number is the ratio of the molecular mean free path λ to a characteristic length scale ℓ, i.e., Kn = λ/ℓ. The inviscid assumption implies that momentum loss due to viscous stresses, heat transfer due to thermal conduction, and viscous diffusion effects are all neglected. The thermodynamics of the inviscid continuum is modeled by treating it as a chemically reactive mixture of thermally perfect gases. The thermal state of the mixture, which may consist of various polyatomic and monatomic species, can be described by a translational-rotational
temperature and a set of vibrational temperatures (or energies), one for each polyatomic species. These temperatures describe the partitioning or distribution of the mixture internal energy among the various allowable molecular energy states. The translational-rotational temperature represents the contribution to the internal energy by the translational and rotational modes of all molecules and atoms in the mixture, which are assumed to be in thermal equilibrium. This is a reasonable approximation for most continuum flow studies as the characteristic time scales for translation-rotational rate processes are very small and the equilibration of the translational-rotational states usually requires very few molecular collisions [Vincenti and Kruger, 1975]. Each vibrational energy represents the contribution to the internal energy by the vibrational modes of the corresponding polyatomic species. Finally, it should be stated that intermolecular forces, electronic excitation, ionization rate processes, and radiation effects are all neglected.

3.2.2 Conservation Equations in Cartesian Coordinates

Under the aforementioned physical assumptions, the weakly conservative forms of the mixture mass, momentum, and energy equations, as well as species mass and vibrational energy equations, governing the flow of the thermally perfect gaseous mixture may be written for a general three-dimensional Cartesian coordinate system as [Vincenti and Kruger, 1975; Anderson, 1982; Anderson, 1989; Gnoffo et al., 1989]

\[ \frac{\partial}{\partial t}(\rho) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(\rho u_i) = 0, \]  
\[ \frac{\partial}{\partial t}(\rho u_i) + \sum_{j \neq i} \frac{\partial}{\partial x_j}(\rho u_i u_j + \delta_{ij} p) = 0, \]  
\[ \frac{\partial}{\partial t}\left[\rho (e_{tr} + e_v + \frac{1}{2} u_i u_i)\right] + \sum_{j} \frac{\partial}{\partial x_j}\left[\rho u_j (e_{tr} + \frac{p}{\rho} + e_v + \frac{1}{2} u_i u_i)\right] = -\rho \sum_{s=1}^{N} w_s \Delta h_{s}^{0}, \]  
\[ \frac{\partial}{\partial t}(\rho c_s) + \sum_{i} \frac{\partial}{\partial x_i}(\rho c_s u_i) = \rho w_s, \quad s = 1, \ldots, N, \]  
\[ \frac{\partial}{\partial t}(\rho c_s e_{v_s}) + \sum_{i} \frac{\partial}{\partial x_i}(\rho c_s e_{v_s} u_i) = \rho c_s q_s + \rho \beta_s w_s e_{v_s}, \quad s = 1, \ldots, N. \]

where the usual tensor notation has been adopted. In Equations (3.1)–(3.5), the independent variables are the time \( t \) and the Cartesian coordinates \( x_i \) (\( i = 1, 2, \) and \( 3 \)), and \( \delta_{ij} \) is the Kronecker delta function. Various dependent variables may be identified. In the PDEs, \( \rho \) is the mixture density, \( u_i \) is the \( i \)-direction velocity, \( p \) is the total pressure of the mixture (i.e., sum of the partial pressures), \( e_{tr} \) is the total specific translational-rotational energy of the mixture, \( c_s = \rho_s / \rho \) is the mass fraction of species \( s \) with \( \sum_s c_s = 1 \), \( \rho_s \) is the density of species \( s \), \( e_{v_s} \) is the specific vibrational energy of species \( s \), \( e_v = \sum_s c_s e_{v_s} \) is the total specific vibrational energy of the mixture, and \( N \) is the number of species in the mixture.

The constant \( \Delta h_{s}^{0} \) is the heat of formation of species \( s \) evaluated at a temperature of absolute zero (0 K), and the source term \( -\rho \sum_s w_s \Delta h_{s}^{0} \) of Eq. (3.3) represents the total change in the zero-point energy of the mixture resulting from chemical reactions. Additionally, the variable \( w_s \) represents the time rate of change of the concentration \( c_s \) of the species \( s \) brought about by the chemical reactions. The variable \( q_s \) represents the time rate of change of the vibrational energy \( e_{v_s} \) of the species \( s \) brought about by relaxation to
its equilibrium value. Finally, the term $\rho \beta_s w_s e_v$ appearing in Eq. (3.5) is related to the change in the vibrational energy of species $s$ per unit volume of the mixture due to the chemical reactions. The parameter $\beta_s$ is an empirical value greater than or equal to unity and is used to reflect an observed preference of higher-than-average vibrationally excited molecules to dissociate and the tendency of atoms to combine and form higher-than-average vibrationally excited molecules [Gnoffo et al., 1989].

It is worth noting that the specification of the quantities $w_s$ and $q_s$ associated with the chemical reaction and vibrational relaxation processes requires a detailed analysis and mathematical modeling of these nonequilibrium physical phenomena for the particular mixture under consideration. The chemical composition, chemical kinetics, reaction mechanisms, and internal energy modes of the mixture must all be considered. A five-species four-temperature nonequilibrium thermodynamic model of air is outlined in Appendix C. This model provides suitable expressions for $w_s$ and $q_s$ in the case of air mixture consisting of five neutral species: nitrogen $N_2$, oxygen $O_2$, nitric oxide NO, and monatomic nitrogen $O$ and oxygen $O$. It is used in all of the nonequilibrium calculations of the present work.

Some additional thermodynamic relationships are useful. The pressure may be expressed in terms of the translational-rotational temperature $T$ or energy $e_{tr}$ and the mixture properties by using the ideal equation of state for each thermally perfect species and applying Dalton's law of partial pressure. The resulting equation of state for the mixture is

$$p = \rho RT = (\gamma - 1)\rho e_{tr},$$

where $R = R(\sum_s c_s / M_s) = \sum_s c_s R_s$ is the specific gas constant of the mixture, $R$ is the universal gas constant, $M_s$ is the molecular weight of species $s$, $R_s = R/M_s$ is the specific gas constant of species $s$, and $\gamma = 1 + [\sum c_s R_s] / [\sum c_s R_s / (\gamma_s - 1)]$ is defined to be the frozen specific heat ratio of the species $s$. Note that these frozen specific heat ratios are the actual specific heat ratio of the species in the absence of vibrational excitation. It is also possible to define a frozen sound speed for the mixture. This intensive property may be related to the other mixture properties by the expression

$$a^2 = \gamma RT = \gamma \frac{p}{\rho} = \gamma (\gamma - 1)e_{tr},$$

where $a$ is the frozen sound speed.

### 3.2.3 Conservation Equations in Two-Dimensional Generalized Curvilinear Coordinates

Aside from the need for a more specific prescription of the source terms, the Euler equations of Eqs. (3.1)–(3.7) provide a complete description of the inviscid flow of the thermochemical nonequilibrium mixture in terms of a general Cartesian coordinate system. However, this study has been confined to two-dimensional planar flows. Furthermore, in many practical applications, it is convenient to solve the governing equations in a transformed or computational coordinate system and relate the conserved and primitive flow variables in the physical domain to their counterparts in the computational space by means of a generalized coordinate transformation. This facilitates the treatment of arbitrary boundaries and readily permits the clustering of grid points in regions of large solution gradients.
Using vector notation, Equations (3.1)-(3.5) may be re-expressed in weak conservation law form for a two-dimensional generalized curvilinear coordinate system as [Anderson et al., 1984; Vinokur, 1974]

$$\frac{\partial}{\partial t}(JU) + \frac{\partial}{\partial \zeta}[F(U)] + \frac{\partial}{\partial \eta}[G(U)] = JS(U),$$  

(3.8)

where the multi-component solution column vector $U$ and source column vector $S$ are given by

$$U = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho[e_tr + e_v + \frac{1}{2}(u^2 + v^2)] \\
\rho c_1 \\
\vdots \\
\rho c_N \\
\rho c_1 e_{v1} \\
\vdots \\
\rho c_N e_{vN}
\end{bmatrix}, \quad S = \begin{bmatrix}
0 \\
0 \\
-\rho \sum_{s=1}^{N} w_s \Delta h_{js} \\
\rho w_1 \\
\vdots \\
\rho w_N \\
\rho c_1 q_1 + \rho \beta_1 w_1 e_{v1} \\
\vdots \\
\rho c_N q_N + \rho \beta_N w_N e_{vN}
\end{bmatrix},$$  

(3.9)

and the $\zeta$- and $\eta$-direction flux column vectors $F$ and $G$ are

$$F = \begin{bmatrix}
\rho U \\
\rho u U + y_\eta p \\
\rho v U - x_\eta p \\
\rho U [e_tr + \frac{p}{\rho} + e_v + \frac{1}{2}(u^2 + v^2)] \\
\rho c_1 U \\
\vdots \\
\rho c_N U \\
\rho c_1 e_{v1} U \\
\vdots \\
\rho c_N e_{vN} U
\end{bmatrix}, \quad G = \begin{bmatrix}
\rho V \\
\rho u V - y_\zeta p \\
\rho v V + x_\zeta p \\
\rho V [e_tr + \frac{p}{\rho} + e_v + \frac{1}{2}(u^2 + v^2)] \\
\rho c_1 V \\
\vdots \\
\rho c_N V \\
\rho c_1 e_{v1} V \\
\vdots \\
\rho c_N e_{vN} V
\end{bmatrix}.$$  

(3.10)

In Eqs. (3.8)-(3.10), $x$ and $y$ are the Cartesian coordinates of the two-dimensional physical space and $u$ and $v$ are the velocity components in this physical coordinate system. The variables $\zeta$ and $\eta$ are the curvilinear coordinates of the transformed or computational space, $x_\zeta = \partial x / \partial \zeta$, $x_\eta = \partial x / \partial \eta$, $y_\zeta = \partial y / \partial \zeta$, $y_\eta = \partial y / \partial \eta$ are the metrics of of the coordinate transformation $x = x(\zeta, \eta)$, $y = y(\zeta, \eta)$, and $J = x_\zeta y_\eta - x_\eta y_\zeta$ is the transformation Jacobian. $U = y_\eta u - x_\zeta v$ and $V = x_\zeta v - y_\eta u$ are the contravariant velocities. A discussion of curvilinear coordinate systems is given in Appendix D. Note that it is usual when referring to the system of conservation laws given by Eq. (3.8) to call $\rho$, $u$, $v$, $p$, $e_tr$, $c_s$, and $e_v$, the primitive dependent variables, whereas, the components of the solution vector $U$ are generally called the conserved dependent variables.
capturing scheme for hyperbolic conservation laws that did not require the explicit addition of artificial dissipation. Lax's method is first-order accurate with the leading term in the truncation error corresponding to the second derivative of the solution and thus, the method is sufficiently dissipative to smooth discontinuities [Anderson et al., 1984]. One significant result of this early work of Lax was that it was demonstrated that a difference method is guaranteed to converge to a weak solution (i.e., shocks represented by smooth transitions propagate with the correct velocity) if the difference scheme is consistent with the conservation form of the PDEs and it converges. What is meant by 'consistent with the conservation form of the PDEs'? This can be understood by considering the hyperbolic conservation laws of Eq. (2.1). For a uniform discretized spatial domain $x_i = i\Delta x$ and $u(i\Delta x, t) = u_i$, where $\Delta x$ is the node point spacing and $i \in [0, 1, \ldots, I]$, a $(2k+1)$-point semi-discrete finite-difference scheme with an appropriate choice of time differencing is said to be consistent with the conservation laws if the solution change $\frac{\partial u}{\partial t}$ can be written in the form [Lax, 1954; Lax and Wendroff, 1960; Harten, 1983; Harten, 1984]

$$\left( \frac{\partial u}{\partial t} \right)_i = \frac{-1}{\Delta x} \left( h_{i+1/2} - h_{i-1/2} \right), \quad (2.5)$$

where $h_{i+1/2}$ is a numerical approximation to the flux at the interface between nodes $i$ and $i+1$ having the form

$$h_{i+1/2} = h(u_i-k+1, \ldots, u_{i+k}), \quad (2.6)$$

that is consistent with the flux function $f(u)$ such that for $u_{i-k+1} = \ldots = u_{i+k} = u$

$$h(u, \ldots, u) = f(u). \quad (2.7)$$

Here, the integer value $k$ defines the spatial bandwidth of the method. Note that one direct consequence of this type of construction for the spatial differencing is that only the boundary fluxes at interfaces $i = 1/2$ and $i = I - 1/2$ contribute to the sum of the flux differences $h_{i+1/2} - h_{i-1/2}$, i.e.,

$$- \Delta x \sum_{i=0}^{I-1} \left( \frac{\partial u}{\partial t} \right)_i = \sum_{i=0}^{I-1} \left( h_{i+1/2} - h_{i-1/2} \right) = h_{I-1/2} - h_{1/2}. \quad (2.8)$$

Hence, methods that are consistent with the convergence form of the PDEs also satisfy a discrete form of the conservation property defined by the integral condition of Eq. (2.3). This is obviously desirable. Schemes of the form of Eq. (2.5) are sometimes termed conservative discretizations [Roe, 1986a].

Another early shock-capturing technique was proposed by Godunov [1959]. This remarkable and original method can be viewed as the first successful conservative upwind scheme as well as the first flux-difference splitting method [Hirsch, 1990]. Like Lax's method, Godunov's solution technique also employs a conservative discretization procedure that is consistent with the divergence form of the conservation laws. However, rather than developing formulas for the interface flux from finite-difference approximations, the method makes use of the exact solution of a local Riemann IVP posed between adjacent nodes $i$ and $i+1$ to evaluate the interface numerical flux function $h_{i+1/2}$. The use of the information from the Riemann problem solution provides Godunov's scheme with the ability to recog-
nize and correctly propagate shocks and other discontinuities as well as makes certain that the method converges to a physically correct generalized solution. Riemann problems and their solution are discussed in Appendix A. Note that the use of the Riemann problem to resolve discontinuities in a shock-capturing method can, in some ways, be regarded as a clever utilization of shock-tracking concepts.

Although not a finite-difference based scheme, an algorithm that is somewhat related to Godunov's method is the random-choice method (RCM) of Glimm [Glimm, 1965; Gottlieb, 1988]. The RCM, which arose from a theoretical existence proof, is a rather unconventional explicit time-marching shock-capturing method for solving systems of hyperbolic equations. Like Godunov's method, it also makes use of the Riemann problem but instead of using a difference formulation to update the solution, the values of the approximate RCM solution at new time levels are obtained by sampling the exact Riemann problem solutions at randomly chosen points within each grid interval. A random number sequence is used to direct the solution sampling and so, in a sense, the RCM may be regarded as a Monte Carlo technique. The important advantages of the method are the sharp resolution of discontinuities and the absence of the usual dissipative and dispersive truncation errors associated with finite-difference and finite-volume methods. In one space dimension, considerable success has been achieved [Gottlieb, 1988; Groth and Gottlieb, 1988; Zhang and Gottlieb, 1986]. Unfortunately, useful extensions of the RCM to more than one spatial dimension have not been forthcoming.

In summary, these first attempts at shock capturing were in fact quite successful. The shock-capturing concept appeared to be justified and the use of a conservative discretization procedure and the Riemann problem were shown to be helpful in ensuring good numerical results. Nevertheless, most of the early finite-difference methods were explicit, three-point, first-order accurate time-marching schemes. Whether by the explicit addition of artificial viscosity or through the inherent (implicit) dissipation introduced by the differing formulation, almost all of these schemes, with the exception of the RCM, were heavily dissipative with strong smearing of discontinuities (see the example calculation of Figure 2.1 and notice particularly the smearing of the contact surface). Therefore, unless excessively refined computational meshes were used, it was generally felt that the solution quality of these first-order methods near shocks was unsatisfactory for many applications, especially nonstationary multi-dimensional problems of gas dynamics. This led to a search for more accurate solution methods.

Before continuing, it should be pointed out that much of the early research into shock-capturing techniques was aided, to a large extent, by the development of the mathematical theory of hyperbolic systems of conservation laws, which matured greatly during the time period. Mathematicians have considerable interest in numerical techniques for they offer the possibility of proving the existence of solutions to IVPs with arbitrary initial data.

### 2.4.2 Higher-Order Finite-Difference Methods

In an effort to improve the accuracy and reduce the grid-point requirements of shock-capturing methods, both explicit and implicit second-order accurate finite-difference representations of hyperbolic conservation laws were investigated during the 1960s and early 1970s. A number of second-order shock-capturing schemes were devised. These included the second-order explicit method of Lax and Wendroff [1960], the explicit predictor-corrector scheme of MacCormack [MacCormack, 1969; MacCormack and Paullay, 1972], the explicit second-order upwind scheme of Warming and Beam [1976], and the implicit centered-
Chapter 4

Upwind TVD Flux-Difference Split Schemes

4.1 Introductory Remarks

The Euler equations governing inviscid compressible two-dimensional planar flow of a thermochemical nonequilibrium thermally perfect gaseous mixture in terms of a generalized curvilinear coordinate system are introduced in the preceding chapter. This nonlinear system of conservation laws, given by Eqs. (3.8)-(3.10), is in weak conservation form and is of the hyperbolic type (i.e., the characteristics are all real). It should be readily apparent that closed-form analytic solutions to general initial boundary value problems (IBVPs) for these equations are not available and numerical solution procedures are therefore necessary. However, the numerical solution of the equations can be problematic.

As with other nonlinear hyperbolic systems, generalized or weak solutions to the Euler equations for thermochemical nonequilibrium flow exist and strong solution discontinuities such as shock waves, contact surfaces, and slipstreams are permitted. For many gaseous mixtures of practical interest, such as high-temperature air, the hyperbolic system can also become rather large, owing to the number of species that must be taken into account. In addition to these complications, the inhomogeneous source terms of Eqs. (3.8)-(3.10) related to the thermal and chemical nonequilibrium rate processes are often large and, in many cases, make solution algorithms stiff (i.e., as in the solution of stiff systems of ordinary differential equations, the time stepping of a marching procedure is drastically constrained by stability considerations rather than by the usual accuracy concerns). These features can make the numerical solution of the nonequilibrium Euler equations rather difficult. Shock resolution and algorithm stability requirements, coupled with the relatively large number of equations to be solved, can place large demands on available computational resources. There is therefore a requirement for accurate, robust, and efficient solution algorithms.

Numerous CFD studies have shown that TVD schemes are very appropriate shock-capturing methods (for evidence of this, refer to the partial review of the literature presented in Chapter 2). In this study, partially-decoupled flux-difference split (FDS) upwind TVD algorithms are proposed for solving the system of hyperbolic conservation laws describing inviscid thermochemical nonequilibrium gaseous flows given in Chapter 3. A semi-implicit time-stepping algorithm is proposed for nonstationary flows and a factored fully implicit procedure is suggested for stationary flow solution. The implicit time-stepping and equation-decoupling techniques utilized by both solution algorithms are helpful in coping with the stiff source terms and size of the governing equations. This chapter is devoted to providing an outline of these FDS upwind TVD methods and includes details of the associated partially-decoupled approach, splitting techniques, approximate Riemann solvers, and
discretization schemes. The semi-implicit scheme is described in Section 4.4 and the fully implicit algorithm is presented in Section 4.5. The equation decoupling and FDS methods are common to both of these methods and are therefore discussed first. Note that, for more efficient solutions of steady-state flow problems, convergence rate enhancement of the factored implicit TVD scheme is sought via a multigrid procedure. The next chapter (Chapter 5) is concerned with the multigrid version of the fully implicit TVD scheme.

4.2 Equation Decoupling: Partially-Decoupled Approach

4.2.1 Gas-Dynamic and Thermodynamic Subsystems

Time-marching upwind TVD finite-difference algorithms are proposed herein for both unsteady and steady solutions to IBVPs for the Euler equations of inviscid thermochemical nonequilibrium flow. However, rather than integrating Eqs. (3.8)-(3.10) simultaneously in a directly coupled solution procedure, the system of hyperbolic conservation laws is partially decoupled and two alternate subsystems are defined: a gas-dynamic and a thermodynamic subsystem. The resulting subsystems are then integrated sequentially in a two-stage time-lagged uncoupled manner. The decoupling technique and associated time-marching (or iterative) algorithm can be defined as follows. Given a solution \( U(\zeta, \eta, t_0) \) of Eq. (3.8) at time \( t_0 \), an approximate numerical solution is obtained at some later time \( t_0 + \Delta t \), where \( \Delta t \) is a small time increment, by first solving a gas-dynamic IBVP defined by

\[
\frac{\partial}{\partial t}(JW) + \frac{\partial}{\partial \zeta}[\dot{F}(W)] + \frac{\partial}{\partial \eta}[\dot{G}(W)] = 0 ,
\]

\[ t_0 < t \leq t_0 + \Delta t , \quad W(\zeta, \eta, t_0) = W(U(\zeta, \eta, t_0)) ,
\]

and then solving a nonequilibrium thermodynamic IBVP given by

\[
\frac{\partial}{\partial t}(JQ) + U \frac{\partial}{\partial \zeta}[H(Q)] + V \frac{\partial}{\partial \eta}[H(Q)] = J\dot{S}(Q) ,
\]

\[ t_0 < t \leq t_0 + \Delta t , \quad Q(x, y, t_0) = Q(W(\zeta, \eta, t_0 + \Delta t), U(\zeta, \eta, t_0)) ,
\]

where the various solution, flux, and source column vectors of the two newly defined subsystems are

\[
W = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho \left[ \frac{p}{\gamma - 1} + e_v + \frac{1}{2}(u^2 + v^2) \right]
\end{bmatrix}, \quad Q = \begin{bmatrix}
c_1 \\
\vdots \\
c_N \\
c_1 e_{v_1} \\
\vdots \\
c_N e_{v_N}
\end{bmatrix} , \quad (4.5)
\]

\[
\rho \left[ \frac{p}{\gamma - 1} + e_v + \frac{1}{2}(u^2 + v^2) \right]
\]

where the various solution, flux, and source column vectors of the two newly defined subsystems are
The approximate solution at $t_0 + \Delta t$ is then given by

$$U(\zeta, \eta, t_0 + \Delta t) \approx U(W(\zeta, \eta, t_0 + \Delta t), Q(\zeta, \eta, t_0 + \Delta t)). \quad (4.8)$$

A solution for all time $t > t_0$ may be obtained by repeating the two-step algorithm and, in the limit of vanishing $\Delta t$, this solution should converge to the exact solution of Equation (3.8). Furthermore, as $t \rightarrow \infty$ a consistent steady-state solution should be obtained.

The seven-component subsystem of Eq. (4.1) is derived by employing a frozen flow assumption and equating the finite-rate thermodynamic source terms of Eq. (3.8) to zero. These equations describe the nonequilibrium solution in the limit as the Damköhler number approaches zero. The behaviour of the mixture is essentially that of a thermally and calorically perfect gas, except that the specific heat ratio and gas constant may vary throughout the flow field and a portion of the internal energy is locked in the vibrational modes. The last three equations of the gas-dynamic subsystem are introduced to include these effects and describe changes in the quantities $\gamma R$, $e_v$, that, in the frozen flow limit, are merely convected with the flow. The use of separate flow equations for describing the evolution of these gas-dynamic quantities is akin to the ideas put forward by Colella and Glaz [1985] for solving equilibrium flows of real gases. In their work, an equation for the convection of an equivalent $\gamma$ was introduced for solving flows of real gases in complete thermodynamic equilibrium.

The multi-component $N$-species thermodynamic subsystem represented by Eq. (4.3) is derived by assuming that $\rho$, $u$, and $v$ are known and fixed. The subsystem describes the time rate of change of the species mass fractions and vibrational energies and the total internal energy and includes the source terms neglected in the derivation of Eq. (4.1). The primitive variables $c_s, e_v$, and $T$, and consequently $e, e_v, p$, and the other thermodynamic properties, are all updated by solving this subsystem.
4.2.2 Comparisons to Chemistry-Split and Fully Coupled Methods

The preceding decoupling procedure is similar in spirit to the techniques put forward by Glaz et al. [1988] and Ben-Artzi [1989] and the resulting subsystems resemble to some extent the uncoupled equation sets that may be obtained by using the equation-partitioning procedure suggested by Yee and Shinn [1989]. In the GRP method of Ben-Artzi for reactive flow, the solution of the homogeneous frozen-flow equations (i.e., source terms set to zero) is used to construct solutions for the fully reactive case. The basic proposition employed is that, for a given IBVP with initial conditions specified at \( t = t_0 \), the inhomogeneous solution can be equated to the homogeneous solution in the limit as \( t \to t_0 \) and that approximations to the reactive flow solution can be derived by applying corrections to the non-reacting solution. This is the essence of the present equation-decoupling technique.

The term "partially decoupled" is applied here to distinguish the current method from fully coupled algorithms, which at each level in a marching procedure solve the complete set of conservation laws in a single step, and from uncoupled, loosely coupled, or chemistry-split techniques, which at each level decouple the gas-dynamic and finite-rate thermodynamic equations and solve them separately in a two-stage process [Yee and Shinn, 1989; Larrouturou, 1991].

The partially-decoupled approach differs from uncoupled or chemistry-split methods because it provides a physically consistent procedure for separating the gas-dynamic and finite-rate models. Furthermore, it will be shown that the decoupling procedure readily permits the use of the eigenvalues and eigenvectors of the complete system in the evaluation of the numerical fluxes of each subsystem. Loosely coupled methods usually employ the eigenvalues and eigenvectors of each decoupled subsystem. The use of the eigenvalues and eigenvectors of the full equations should enhance the coupling between the equation sets and thereby improve numerical solution quality [Yee and Shinn, 1989]. It can also be shown that if the numerical solutions of Eqs. (4.1) and (4.3) are constructed using the proposed TVD schemes and flux-difference splitting procedures of this chapter, then the approximate solutions preserve discrete forms of the monotonicity, positivity, and maximum principles for the mass fractions of each species \( c_s \) as defined by Larrouturou [1991] without requiring the solution of the fully coupled conservation laws (see Section 4.4.5). These principles ensure that \( 0 \leq c_s \leq 1 \) and \( \sum_s c_s = 1 \), which are two conditions that must be satisfied for physically realistic solutions. Larrouturou points out that chemistry-split and FDS fully coupled solution schemes do not always satisfy these important principles and further suggests a possible remedy for the FDS fully coupled schemes.

The primary advantages of the present decoupling procedure as compared to fully coupled methods are related to its simplicity and computational efficiency. One solver can be developed for the gas-dynamic subsystem of the partially-decoupled approach and used to predict the flow of many different nonequilibrium gaseous mixtures. Mixture-specific solvers are needed only for the thermodynamic subsystem. This simplifies computer program development and enhances algorithm versatility. Furthermore, with the partially-decoupled approach (as with chemistry-split methods), it is easy to employ local-time-stepping or subiteration procedures for solving the thermodynamic subsystem without changing the integration of the gas-dynamic subsystem. It is also easy to utilize different solvers for the thermodynamic subsystem in different regions of the flow depending on the solution characteristics. This additional capability makes the approach more flexible and may be useful for treating cases where the source terms are very stiff [LeVeque and Yee, 1990].

The present decoupling technique can also lead to significant computational savings.
when fully implicit schemes are used to solve the gas-dynamic and thermodynamic sub-
systems. Although three additional equations must be solved for $\gamma$, $R$, and $e_v$, the reduced
subsystems are of sizes 7 and $2N + 1$ as compared to the complete system that is of size
$2N + 4$. In addition, it will be shown that for linearized factored implicit algorithms the
solution of the inviscid thermodynamic subsystem does not require the inversion of full
$(2N + 1) \times (2N + 1)$ block tridiagonal systems. In at least one sweep direction, it is only
necessary to invert $2N$ scalar tridiagonal systems. In the other sweep direction, the subma-
trices of the off-diagonal blocks contain only diagonal elements and simple diagonalization
procedures are possible. For large systems, these features may be exploited to reduce the
number of operation counts associated with each iteration of an implicit solution procedure.

In some cases, the explicit coupling of gas-dynamic and finite-rate subsystems provided
by the partial-decoupling procedure may not be adequate for numerical predictions of steady,
viscous, combusting flows. Fully coupled algorithms with implicit coupling may be more
efficient. However, for many applications, such as those considered in following chapters,
the partially-decoupled approach is valid and performs well. The technique has been applied
successively by Groth et al. [1991] to predict one-dimensional nonstationary nonequilibrium
flow in a hypersonic impulse tunnel (see Appendix B).

4.3 Flux-Difference Splitting and
Approximate Riemann Solvers

Having uncoupled the gas-dynamic and thermodynamic equations as described above, the
two subsystems can be updated at each time (or iteration) level by means of a TVD finite-
difference method. As TVD schemes were originally developed for solving linear and non-
linear scalar homogeneous hyperbolic conservation laws in one space dimension, algorithm
extensions are necessary for these weakly conservative two-dimensional subsystems. The
extension to two dimensions is achieved herein by dimension splitting. The nonlinear and
vector nature of the decoupled conservation laws is handled by adopting the characteristic
decomposition or flux-difference splitting technique of Roe [1981] in which the properties of
the flux Jacobians are utilized in conjunction with approximate Riemann solvers to repre-
sent the solution and flux vector jumps in terms of characteristic variables. The flux-vector
splitting techniques of Steger and Warming [1981] and van Leer [1982] are also suitable
for these purposes and offer certain advantages; however, it was felt that flux-difference
splitting affords superior resolution of discontinuities and complex flow features (e.g., [Mul-
der and van Leer, 1985; Liou and van Leer, 1988]) and is therefore used in the proposed
semi-implicit and fully implicit solution schemes.

Note that the study of Liou and van Leer [1988] compares the various splitting pro-
cedures and demonstrates the superior accuracy of Roe-type FDS schemes. Their study
also shows, as others have found in some cases [Mulder and van Leer, 1985; Yee, 1987b;
Yee et al., 1990; Roberts, 1990], that, unlike the other splitting methods, Roe-type FDS
can have poor convergence rates and exhibit limit-cycle behaviour when implemented in
implicit time-marching or relaxation schemes for steady-state flow calculations. This has
been shown to be particularly true when higher-order spatial discretization methods are
employed. Some causes for these convergence problems are offered later in the chapter.
4.3.1 Eigensystems of Flux Jacobian Matrices

The homogeneous terms of the thermodynamic subsystem represent pure convection and the partial differential equations are therefore already in characteristic form. A decomposition procedure is however required for the gas-dynamic subsystem. Following Glaister [1988a; 1988b; 1988d], extensions to Roe's approximate Riemann solver have been developed (see Section 4.3.2) and are used in the evaluation of the numerical flux functions for Eq. (4.1) to account for the transformed coordinate system and the effects of varying $\gamma$ and $R$ and non-zero $\epsilon_v$. These approximate Riemann solutions require information about the eigensystems of the flux Jacobians $\mathbf{A} = \partial \mathbf{F} / \partial \mathbf{W}$ and $\mathbf{B} = \partial \mathbf{G} / \partial \mathbf{W}$.

It can be shown (see Appendix A) that the seven eigenvalues and right eigenvectors of the $\zeta$-direction flux Jacobian satisfying $\mathbf{A} \mathbf{e}_k = \lambda_k \mathbf{e}_k$, $k = 1, \ldots, 7$, are

$$
\lambda_1 = U - a \sqrt{x_\eta^2 + y_\eta^2}, \quad \lambda_7 = U + a \sqrt{x_\eta^2 + y_\eta^2},
$$

$$
\lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = \lambda_6 = y_\eta u - x_\eta v = U, \quad (4.9)
$$

$$
e_1 = \begin{bmatrix}
u - \frac{1}{y_\eta} a \\
\frac{\sqrt{x_\eta^2 + y_\eta^2}}{x_\eta a} \\
\frac{\sqrt{x_\eta^2 + y_\eta^2}}{a U} \\
\gamma \\
\gamma R \\
e_v
\end{bmatrix}, \quad e_2 = \begin{bmatrix}
u + \frac{1}{2} (u^2 + v^2) \\
\frac{1}{u} \\
\frac{v}{\gamma} \\
R \\
\gamma R \\
e_v
\end{bmatrix}, \quad e_7 = \begin{bmatrix}
u - \frac{1}{y_\eta} a \\
\frac{\sqrt{x_\eta^2 + y_\eta^2}}{x_\eta a} \\
\frac{\sqrt{x_\eta^2 + y_\eta^2}}{a U} \\
\gamma \\
\gamma R \\
e_v
\end{bmatrix}, \quad (4.10)
$$

$$
e_3 = \begin{bmatrix}0 \\
x_\eta \\
y_\eta \\
0 \\
0 \\
0
\end{bmatrix}, \quad e_4 = \begin{bmatrix}0 \\
0 \\
0 \\
\frac{-a^2}{(\gamma - 1)^2} \\
\gamma \\
0
\end{bmatrix}, \quad e_5 = \begin{bmatrix}0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{bmatrix}, \quad e_6 = \begin{bmatrix}0 \\
e_v \\
0 \\
0 \\
0 \\
e_v
\end{bmatrix}, \quad (4.11)
$$

where $h$ is the specific enthalpy of the mixture and is given by

$$
h = e_{tr} + \frac{p}{\rho} + e_v + \frac{1}{2} (u^2 + v^2) = \frac{\gamma p}{(\gamma - 1)\rho} + e_v + \frac{1}{2} (u^2 + v^2). \quad (4.12)
$$

Similar expressions can be obtained for the flux Jacobian $\mathbf{B}$ that satisfy $\mathbf{B} \mathbf{e}_k = \lambda_k \mathbf{e}_k$. The eigenvalues and eigenvectors are

$$
\lambda_1 = V - a \sqrt{x_\zeta^2 + y_\zeta^2}, \quad \lambda_7 = V + a \sqrt{x_\zeta^2 + y_\zeta^2},
$$

$$
\lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = \lambda_6 = x_\zeta v - y_\zeta u = V, \quad (4.13)
$$

$$
\lambda_1 = V - a \sqrt{x_\zeta^2 + y_\zeta^2}, \quad \lambda_7 = V + a \sqrt{x_\zeta^2 + y_\zeta^2},
$$

$$
\lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = \lambda_6 = x_\zeta v - y_\zeta u = V, \quad (4.14)
$$

$$
\lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = \lambda_6 = x_\zeta v - y_\zeta u = V, \quad (4.15)
$$

4.6
Note that \( \hat{A} \) and \( \hat{B} \) have only three distinct eigenvalues. The \( k = 1 \) and 7 characteristic fields of both matrices are genuinely nonlinear in the sense of Lax [1973] (i.e., \( \partial \lambda_k / \partial W \cdot e_k \neq 0 \)), whereas the \( k = 2, 3, 4, 5, \) and 6 eigenvalues and eigenvectors are linearly degenerate and are associated with purely convective fluxes. In addition, the unique eigenvalues of the gas-dynamics subsystem are identical to the unique eigenvalues of the fully coupled conservation laws of Eq. (3.8). This is exploited when constructing the approximate TVD solutions of the next sections.

### 4.3.2 Approximate Riemann Solvers

The key ingredient in the flux-difference splitting approach of Roe is the approximate Riemann solver. It provides a non-iterative characteristic decomposition of the flux Jacobians with shock-recognition features [Roe, 1981]. Following Glaister [1988a; 1988b; 1988d], Roe-type approximate Riemann solvers for the conservation equations of the gas dynamic subsystem can be obtained using the flux Jacobian eigensystem information of the previous subsection. As mentioned earlier, extended versions of Roe's original solver are necessary for the hyperbolic subsystem of Eq. (4.1). This is to account for the generalized curvilinear coordinate system and additional PDEs describing the convection of \( \gamma, R, \) and \( e_v. \) The theory and derivation of the approximate solvers for this frozen-flow case are described in some detail in Appendix A. Please refer to this appendix for additional information. Along with the equation decoupling technique of Section 4.2, these extended approximate Riemann solutions are used by the proposed FDS upwind TVD schemes for the solution of the Euler equations for thermochemical nonequilibrium flows which now follow.

### 4.4 Semi-Implicit TVD Scheme

Using the proposed equation decoupling technique, finite-difference solutions of Eq. (3.8) can be obtained by solving the gas-dynamic and thermodynamic subsystems of Eqs. (4.1)
and (4.3) alternately in a time-lagged fashion. A semi-implicit TVD scheme is proposed for time-accurate numerical solutions. The implicit time differencing of the source terms modeling the finite-rate processes effectively alleviates the stiffness associated with the relaxation and reaction time scales. The explicit treatment of the inviscid fluxes is generally quite efficient for unsteady applications. For the present study, the higher-order TVD upwind flux-differencing scheme of Roe [Roe, 1981; Roe and Pike, 1984; Sweby, 1984; Sweby and Baines, 1984] is used as the underlying scalar solver. Like other TVD methods the scheme is a smart solution adaptive method that provides improved numerical accuracy and monotonic or oscillation-free solutions by having difference coefficients which depend on the local solution at each time step. The unlimited constant-coefficient scheme is a combination of the second-order schemes of Lax and Wendroff [1960] (central differences) and Warming and Beam [1976] (upwind differences). Flux limiters [Sweby, 1984] are employed to limit the magnitude of the second-order antidiffusive fluxes and reduce the scheme to the first-order fully-upwind method of Cole and Murman [Murman, 1974] at local extrema of the solution. The extension to two dimensions is achieved by the usual Strang-splitting or operator-splitting method [Strang, 1968; Colella, 1990], in which the one-dimensional algorithm is applied to the one-dimensional analogues of the multi-dimensional equation sets in both coordinate directions. The approximate Riemann solvers of Appendix A are employed to decompose solution and flux vectors of the time-split conservation laws, which are then solved by applying explicit and semi-implicit versions of Roe's scheme to each characteristic field in a scalar fashion.

As with other TVD schemes, the term “higher-order” is applied to Roe's method to indicate that the formal spatial accuracy of the scheme with a uniform computational mesh is second-order in regions where the solution is smooth (i.e., almost everywhere), but reduces to first-order at extrema. In the case of linear and nonlinear scalar homogeneous hyperbolic conservation laws and linear systems of homogeneous conservation laws in one space dimension, the resulting nonlinear scheme is TVD [Harten, 1983; Harten, 1984], which guarantees that the solutions are also monotonicity preserving. Further to this, Sweby and Baines [1984] have demonstrated that the scheme of Roe converges to weak, although not necessarily unique, solutions for the nonlinear scalar wave equation and discuss appropriate corrections for the removal of entropy-violating shocks. In the more general case of nonlinear multidimensional systems the accuracy and TVD properties may not be realized. Firstly, the truncation error in the physical space can be achieved only when the coordinate transformation is smooth [Thompson et al., 1985]. Furthermore, the notion of what constitutes a TVD solution in two space dimensions remains largely unresolved. However, the recent work of Colella [1990] indicates that operator split methods have the same resolution as unsplit methods and many other numerical experiments indicate that higher-order TVD techniques afford improved solution accuracy.

4.4.1 Discretized Equations

The proposed semi-implicit algorithm can be formulated as follows. Let \( U_{i,j}^n \) be the numerical approximation of the solution of Eq. (3.8) at time \( t = t^n \) and at discrete locations \((i, j)\), with curvilinear coordinates \((\zeta_i, \eta_j)\). The numerical solution at subsequent time levels is

\textsuperscript{1}Goodman and LeVeque [1985] argue that time-split TVD algorithms applied to two-dimensional systems are, at most, first-order accurate. However, their paper is somewhat confusing and does not appear to truly clarify the issue of TVD solutions for the multidimensional case.
obtained by means of the fully-discrete time-stepping procedure

$$U_{i,j}^{n+1} = L_{W_t}^{i,j} L_{Q_t}^{i,j} L_{W}^{i,j} L_{Q}^{i,j} U_{i,j}^{n} ,$$  \hspace{1cm} (4.18)$$

with $\Delta t^n = t^{n+1} - t^n$, and where the gas-dynamic and thermodynamic subsystem solution operators are

$$L_{W_t}^{i,j} U_{i,j}^{n} = U(W_{i,j}^{n+1}, Q_{i,j}^{n}) ; \quad \Delta W_{i,j}^{n} = W_{i,j}^{n+1} - W_{i,j}^{n} =$$

$$-\frac{1}{2} \sum_{k=1}^{7} \left\{ \left( \nu_{i,j+1/2,k}^{n} - \nu_{i,j+1/2,k}^{n+1} \right) + \phi_{i,j+1/2,k}^{n} \nu_{i,j+1/2,k}^{n+1} (1 - \nu_{i,j+1/2,k}^{n}) \right\} \Delta W_{i,j}^{n},$$

$$+ \left\{ \left( \nu_{i,j-1/2,k}^{n} - \nu_{i,j-1/2,k}^{n+1} \right) + \phi_{i,j-1/2,k}^{n} \nu_{i,j-1/2,k}^{n+1} (1 - \nu_{i,j-1/2,k}^{n}) \right\} \Delta W_{i,j}^{n},$$

$$\Delta W_{i,j}^{n} = W_{i,j}^{n+1} - W_{i,j}^{n}.$$  \hspace{1cm} (4.19)$$

$$L_{W_t}^{i,j} U_{i,j}^{n} = U(W_{i,j}^{n+1}, Q_{i,j}^{n}) ; \Delta W_{i,j}^{n} = W_{i,j}^{n+1} - W_{i,j}^{n} =$$

$$-\frac{1}{2} \sum_{k=1}^{7} \left\{ \left( \nu_{i,j+1/2,k}^{n} - \nu_{i,j+1/2,k}^{n+1} \right) + \phi_{i,j+1/2,k}^{n} \nu_{i,j+1/2,k}^{n+1} (1 - \nu_{i,j+1/2,k}^{n}) \right\} \Delta W_{i,j}^{n},$$

$$+ \left\{ \left( \nu_{i,j-1/2,k}^{n} - \nu_{i,j-1/2,k}^{n+1} \right) + \phi_{i,j-1/2,k}^{n} \nu_{i,j-1/2,k}^{n+1} (1 - \nu_{i,j-1/2,k}^{n}) \right\} \Delta W_{i,j}^{n},$$

$$\Delta W_{i,j}^{n} = W_{i,j}^{n+1} - W_{i,j}^{n}.$$  \hspace{1cm} (4.20)$$

$$L_{Q_t}^{i,j} U_{i,j}^{n} = U(W_{i,j}^{n}, Q_{i,j}^{n+1}) ; \quad \Delta Q_{i,j}^{n} = \Delta t^n \frac{\partial S}{\partial Q}_{i,j}^{n} =$$

$$-\frac{1}{2} \sum_{k=1}^{2N+1} \left\{ \left( \omega_{i,j+1/2,k}^{n} - \omega_{i,j+1/2,k}^{n+1} \right) + \psi_{i,j+1/2,k}^{n} \omega_{i,j+1/2,k}^{n+1} (1 - \omega_{i,j+1/2,k}^{n}) \right\} \Delta H_{i,j}^{n},$$

$$+ \left\{ \left( \omega_{i,j-1/2,k}^{n} - \omega_{i,j-1/2,k}^{n+1} \right) + \psi_{i,j-1/2,k}^{n} \omega_{i,j-1/2,k}^{n+1} (1 - \omega_{i,j-1/2,k}^{n}) \right\} \Delta H_{i,j-1/2,k}^{n},$$

$$\Delta Q_{i,j}^{n} = Q_{i,j}^{n+1} - Q_{i,j}^{n}.$$  \hspace{1cm} (4.21)$$

$$L_{Q_t}^{i,j} U_{i,j}^{n} = U(W_{i,j}^{n}, Q_{i,j}^{n+1}) ; \quad \Delta Q_{i,j}^{n} = Q_{i,j}^{n+1} - Q_{i,j}^{n} =$$

$$-\frac{1}{2} \sum_{k=1}^{2N+1} \left\{ \left( \omega_{i,j+1/2,k}^{n} - \omega_{i,j+1/2,k}^{n+1} \right) + \psi_{i,j+1/2,k}^{n} \omega_{i,j+1/2,k}^{n+1} (1 - \omega_{i,j+1/2,k}^{n}) \right\} \Delta H_{i,j}^{n},$$

$$+ \left\{ \left( \omega_{i,j-1/2,k}^{n} - \omega_{i,j-1/2,k}^{n+1} \right) + \psi_{i,j-1/2,k}^{n} \omega_{i,j-1/2,k}^{n+1} (1 - \omega_{i,j-1/2,k}^{n}) \right\} \Delta H_{i,j-1/2,k}^{n},$$

$$\Delta Q_{i,j}^{n} = Q_{i,j}^{n+1} - Q_{i,j}^{n}.$$  \hspace{1cm} (4.22)$$

and \Delta W_{i,j}^{n} = W_{i,j}^{n+1} - W_{i,j}^{n} ; \quad \Delta Q_{i,j}^{n} = Q_{i,j}^{n+1} - Q_{i,j}^{n} ; \quad \Delta W_{i,j}^{n+1} and \Delta Q_{i,j}^{n+1} denote intermediate solution states. Note that the superscript $n$ refers to the $n$th time level $t^n$, the subscripts $i$ and $j$ imply quantities evaluated at node $(i,j)$, and the subscript $k$ relates to the $k$th characteristic field. In most cases, the subscripts $i+1/2,j$ and $i,j+1/2$ refer to averaged quantities at the nodal interfaces between the grid points $(i,j)$ and $(i+1,j)$ and $(i,j)$ and $(i,j+1)$, respectively.

In Eq. (4.21), $I$ is the identity matrix, $\partial S/\partial Q$ is the source Jacobian matrix, and the
term \([I - \Theta \Delta t^n (\partial \dot{S}/\partial \mathbf{Q})_{i,j}^n]\) is similar to the preconditioning matrices used by Bussing and Murman [1988]. The parameter \(\Theta\) controls the time integration of the source terms of the operator \(L_{ij}^n\). For \(\Theta = 0\) the time differencing is Euler explicit. For \(\Theta = 1\) the time differencing is Euler implicit; this value produces the most stable scheme and is appropriate for problems with extremely stiff source terms. A value of \(\Theta = 1/2\) produces a trapezoidal implicit time differencing that is best suited for and consistent with the explicit time-differencing of the homogeneous terms.

The quantities \(\nu_{i+1/2,j,k}^n\) and \(\Delta \mathbf{W}_{i+1/2,j,k}^n\) appearing in Eq. (4.19) are the local average Courant-Friedrichs-Lewy (CFL) number and solution jump vector for the \(k\)th elemental wave of the gas-dynamic subsystem spatial operator \(L_{ij}^n\). Similarly, \(\nu_{i,j+1/2,k}^n\) and \(\Delta \mathbf{W}_{i,j+1/2,k}^n\) of Eq. (4.20) are the corresponding CFL number and solution jump vector for the \(L_{ij}^n\) spatial operator. The CFL numbers and solution jump vectors are given by

\[
\nu_{i+1/2,j,k}^n = \frac{\Delta t^n \lambda_{i+1/2,j,k}^n}{J_{i+1/2,j} \Delta \zeta_{i+1/2,j}}, \quad \nu_{i,j+1/2,k}^n = \frac{\Delta t^n \lambda_{i,j+1/2,k}^n}{J_{i,j+1/2} \Delta \eta_{i,j+1/2}},
\]

\[
\Delta \mathbf{W}_{i+1/2,j,k}^n = \alpha_{i+1/2,j,k}^n e_{i+1/2,j,k}^n, \quad \Delta \mathbf{W}_{i,j+1/2,k}^n = \alpha_{i,j+1/2,k}^n e_{i,j+1/2,k}^n,
\]

where \(\Delta \zeta_{i+1/2,j} = \zeta_{i+1,j} - \zeta_{i,j}, \Delta \eta_{i,j+1/2} = \eta_{i,j+1} - \eta_{i,j}\), and where the required transformation metrics \(x_{n_{i+1/2,j}}, y_{n_{i+1/2,j}}, x_{\zeta_{i+1/2,j}}, y_{\zeta_{i+1/2,j}}\), and \(x_{\eta_{i,j+1/2}}, y_{\eta_{i,j+1/2}}\) and Jacobians \(J_{i+1/2,j}\) and \(J_{i,j+1/2}\) may be approximated by standard second-order central finite-difference relations. The metrics are evaluated using the following difference expressions:

\[
x_{n_{i+1/2,j}} = \frac{1}{2} \left( \frac{x_{i+1,j} - x_{i,j-1}}{\Delta \eta_{i,j+1/2} + \Delta \eta_{i,j-1/2}} + \frac{x_{i+1,j+1} - x_{i+1,j-1}}{\Delta \eta_{i,j+1/2} + \Delta \eta_{i,j-1/2}} \right),
\]

\[
y_{n_{i+1/2,j}} = \frac{1}{2} \left( \frac{y_{i+1,j} - y_{i,j-1}}{\Delta \eta_{i,j+1/2} + \Delta \eta_{i,j-1/2}} + \frac{y_{i+1,j+1} - y_{i+1,j-1}}{\Delta \eta_{i,j+1/2} + \Delta \eta_{i,j-1/2}} \right),
\]

\[
x_{\zeta_{i,j+1/2}} = \frac{1}{2} \left( \frac{x_{i+1,j} - x_{i-1,j}}{\Delta \zeta_{i+1/2,j} + \Delta \zeta_{i-1/2,j}} + \frac{x_{i+1,j+1} - x_{i+1,j-1}}{\Delta \zeta_{i+1/2,j} + \Delta \zeta_{i-1/2,j}} \right),
\]

\[
y_{\zeta_{i,j+1/2}} = \frac{1}{2} \left( \frac{y_{i+1,j} - y_{i-1,j}}{\Delta \zeta_{i+1/2,j} + \Delta \zeta_{i-1/2,j}} + \frac{y_{i+1,j+1} - y_{i-1,j+1}}{\Delta \zeta_{i+1/2,j} + \Delta \zeta_{i-1/2,j}} \right),
\]

and the equations

\[
J_{i+1/2,j} = \left( \frac{x_{i+1,j} - x_{i,j}}{\Delta \zeta_{i+1/2,j}} \right) y_{n_{i+1/2,j}} - x_{n_{i+1/2,j}} \left( \frac{y_{i+1,j} - y_{i,j}}{\Delta \zeta_{i+1/2,j}} \right),
\]

\[
J_{i,j+1/2} = x_{\zeta_{i,j+1/2}} \left( \frac{y_{i,j+1} - y_{i,j}}{\Delta \eta_{i,j+1/2}} \right) - \left( \frac{x_{i,j+1} - x_{i,j}}{\Delta \eta_{i,j+1/2}} \right) y_{\zeta_{i,j+1/2}},
\]

are used to determine the interface or average values for the transformation Jacobian. Note that in most computations, it is normally assumed that \(\Delta \zeta_{i+1/2,j} = \Delta \zeta_{i,j+1/2} = 1\).

In Eqs. (4.23) and (4.24), \(\lambda_{i+1/2,j,k}^n\) and \(e_{i+1/2,j,k}^n\) are the \(k\)th eigenvalue and eigenvector of the \(\zeta\)-direction gas-dynamic flux Jacobian \(\dot{\mathbf{A}}\) evaluated at an appropriate average state \(\mathbf{W}_{i+1/2,j,k}^n\). They are defined by \(\lambda_{i+1/2,j,k}^n = \lambda_k^i(W_{i+1/2,j,k}^n)\) and \(e_{i+1/2,j,k}^n = e_k^i(W_{i+1/2,j,k}^n)\) where \(\lambda_k\) and \(e_k\) are given by Eqs. (4.9)-(4.12). Similarly, \(\lambda_{i,j+1/2,k}^n\) and \(e_{i,j+1/2,k}^n\) are
the related eigenvalue and eigenvector for the $\eta$-direction flux Jacobian $\mathbf{B}$ evaluated at $W^{|i+1/2,k}$. They are defined by $
abla_i^{j+1/2,k} = \lambda_k(W^{|i+1/2,k})$ and $e_i^{j+1/2,k} = e_k(W^{|i+1/2,k})$ where $\lambda_k$ and $e_k$ are given by Eqs. (4.14)-(4.17). The variables $\alpha^{i+1/2,j,k}$ and $\beta^{i+1/2,j,k}$ are defined to be the elemental or characteristic wave strengths also evaluated at the local average states $W^{|i+1/2,j,k}$ and $W^{|i+1/2,j,k}$, respectively. The extended Roe-type approximate Riemann solvers of Appendix A for the subsystem of Eq. (4.1) yields expressions for the wave strengths and various dependent variables defining the appropriate average states. The wave strengths of the $\mathcal{C}^{ij}$ spatial operator satisfying the conditions $\Delta W^{|i+1/2,j} = W^{|i+1/2,j} - W^{|i+1/2,j} = \sum_k \Delta W^{|i+1/2,j,k} = \sum_k \alpha^{i+1/2,j,k} e^{i+1/2,j,k}$ and $\Delta \hat{F}^{|i+1/2,j} = \hat{F}^{|i+1/2,j} - \hat{F}^{|i+1/2,j} = \sum_k \Delta \hat{F}^{|i+1/2,j,k}$ are

$$\alpha_{i+1/2,j,1} = \frac{1}{2(a_{i+1/2,j})^2} \left[ \Delta p_{i+1/2,j} - \rho_{i+1/2,j} \alpha_{i+1/2,j} \frac{y_{n+1/2,j} \Delta u_{i+1/2,j} - x_{n+1/2,j} \Delta v_{i+1/2,j}}{\sqrt{x_{n+1/2,j}^2 + y_{n+1/2,j}^2}} \right],$$

$$\alpha_{i+1/2,j,2} = \Delta \rho_{i+1/2,j} - \frac{\Delta p_{i+1/2,j}}{(a_{i+1/2,j})^2},$$

$$\alpha_{i+1/2,j,3} = \rho_{i+1/2,j} \frac{x_{n+1/2,j} \Delta u_{i+1/2,j} + y_{n+1/2,j} \Delta v_{i+1/2,j}}{x_{n+1/2,j}^2 + y_{n+1/2,j}^2},$$

$$\alpha_{i+1/2,j,4} = \frac{\rho_{i+1/2,j}}{\gamma_{i+1/2,j}} \Delta \gamma_{i+1/2,j},$$

$$\alpha_{i+1/2,j,5} = \frac{\rho_{i+1/2,j}}{R_{i+1/2,j}} \Delta R_{i+1/2,j},$$

$$\alpha_{i+1/2,j,6} = \frac{\rho_{i+1/2,j}}{e_{v_{i+1/2,j}}} \Delta e_{v_{i+1/2,j}},$$

$$\alpha_{i+1/2,j,7} = \frac{1}{2(a_{i+1/2,j})^2} \left[ \Delta p_{i+1/2,j} + \rho_{i+1/2,j} \alpha_{i+1/2,j} \frac{y_{n+1/2,j} \Delta u_{i+1/2,j} - x_{n+1/2,j} \Delta v_{i+1/2,j}}{\sqrt{x_{n+1/2,j}^2 + y_{n+1/2,j}^2}} \right],$$

and

$$\rho_{i+1/2,j} = \sqrt{\rho_{i+1/2,j}^2},$$

$$Z_{i+1/2,j}^n = \frac{\sqrt{\rho_{i+1/2,j}^n} Z_{i+1/2,j}^n + \sqrt{\rho_{i+1/2,j}^n} Z_{i+1/2,j}^n}{\sqrt{\rho_{i+1/2,j}^n} + \sqrt{\rho_{i+1/2,j}^n}}, \quad Z = u, v, \gamma, R, e_v, \text{ and } h,$$

$$\nabla_{i+1/2,j} = \left( \gamma_{i+1/2,j} - 1 \right) \left[ h_{i+1/2,j} - e_{i+1/2,j} - \frac{1}{2} \left( (u_{i+1/2,j})^2 + (v_{i+1/2,j})^2 \right) \right],$$

are approximate expressions for the averages of the primitive variables defining $W^{|i+1/2,j,k}$.  

4.11
Similarly, the wave strengths of the $L_{i,j}^{\Delta t}$ spatial operator satisfying the solution and flux jump conditions $\Delta W_{i,j+1/2}^n = W_{i,j+1}^n - W_{i,j}^n = \sum_k \Delta W_{i,j+1/2,k}^n = \sum_k \alpha_{i,j+1/2,k}^n \Delta W_{i,j+1/2,k}^n$ and $\Delta F_{i,j+1}^n = F_{i,j+1}^n - F_{i,j}^n = \sum_k \gamma_{i,j+1/2,k}^n \Delta W_{i,j+1/2,k}^n$ are

$$\alpha_{i,j+1/2,1}^n = \frac{1}{2(a_{i,j+1/2}^n)^2} \left[ \frac{\Delta \rho_{i,j+1/2}^n - \rho_{i,j+1/2}^n a_{i,j+1/2}^n x_{\zeta_{i,j+1/2}}^n \Delta u_{i,j+1/2}^n - y_{\zeta_{i,j+1/2}}^n \Delta u_{i,j+1/2}^n}{\sqrt{x_{\zeta_{i,j+1/2}}^2 + y_{\zeta_{i,j+1/2}}^2}} \right],$$

(4.41)

$$\alpha_{i,j+1/2,2}^n = \Delta \rho_{i,j+1/2}^n - \frac{\Delta \rho_{i,j+1/2}^n}{(a_{i,j+1/2}^n)^2},$$

(4.42)

$$\alpha_{i,j+1/2,3}^n = \rho_{i,j+1/2}^n \frac{x_{\zeta_{i,j+1/2}}^n \Delta u_{i,j+1/2}^n + y_{\zeta_{i,j+1/2}}^n \Delta u_{i,j+1/2}^n}{x_{\zeta_{i,j+1/2}}^2 + y_{\zeta_{i,j+1/2}}^2},$$

(4.43)

$$\alpha_{i,j+1/2,4}^n = \frac{\rho_{i,j+1/2}^n}{\gamma_{i,j+1/2}^n} \Delta \gamma_{i,j+1/2}^n,$$

(4.44)

$$\alpha_{i,j+1/2,5}^n = \frac{\rho_{i,j+1/2}^n}{R_{i,j+1/2}^n} \Delta R_{i,j+1/2}^n,$$

(4.45)

$$\alpha_{i,j+1/2,6}^n = \frac{\rho_{i,j+1/2}^n}{e_{i,j+1/2}^n} \Delta e_{i,j+1/2}^n,$$

(4.46)

$$\alpha_{i,j+1/2,7}^n = \frac{1}{2(a_{i,j+1/2}^n)^2} \left[ \frac{\Delta \rho_{i,j+1/2}^n + \rho_{i,j+1/2}^n a_{i,j+1/2}^n x_{\zeta_{i,j+1/2}}^n \Delta u_{i,j+1/2}^n - y_{\zeta_{i,j+1/2}}^n \Delta u_{i,j+1/2}^n}{\sqrt{x_{\zeta_{i,j+1/2}}^2 + y_{\zeta_{i,j+1/2}}^2}} \right],$$

(4.47)

and the average solution state $\bar{W}_{i,j+1/2,k}^n$ is defined by expressions with forms identical to Eqs. (4.38)–(4.31). Note that for Eqs. (4.31)–(4.37) and (4.41)–(4.47), the notation $\Delta Z_{i,j+1/2}^n = Z_{i,j+1}^n - Z_{i,j}^n$ and $\Delta Z_{i,j+1/2}^n = Z_{i,j+1}^n - Z_{i,j}^n$ is assumed.

In the discrete difference expressions of Eqs. (4.21) and (4.22) for the solution of the thermodynamic subsystem, $\omega_{i,j+1/2,j}^n$ and $\omega_{i,j+1/2}^n$ are the local CFL numbers and $\Delta H_{i,j+1/2,k}^n$ and $\Delta H_{i,j+1/2,k}^n$ are the species concentration and vibrational energy jump column vectors of the spatial operators $L_{i,j}^{\Delta t}$ and $L_{i,j}^{\Delta t}$. The CFL numbers can be expressed as

$$\omega_{i,j+1/2,j}^n = \frac{\Delta \omega_{i,j+1/2,j}^n}{J_{i,j+1/2,j}^n \Delta \zeta_{i,j+1/2,j}^n}, \quad \omega_{i,j+1/2}^n = \frac{\Delta \omega_{i,j+1/2}^n}{J_{i,j+1/2}^n \Delta \eta_{i,j+1/2}^n},$$

(4.48)

where $U_{i,j+1/2,j}^n$ and $V_{i,j+1/2}^n$ are the local average convection velocities. The average convection velocities are determined by using the eigenvalues associated with the linear fields of the gas-dynamic subsystem and are specified as follows: $U_{i,j+1/2,j}^n = \lambda_{i,j+1/2,j}^n$ and $V_{i,j+1/2}^n = \lambda_{i,j+1/2}^n$. In this way, the eigenvalues of the fully coupled system are used in the computation of the flux functions of both the gas-dynamic and thermodynamic subsystems. The solution jumps for the $N_D = 2N + 1$ component thermodynamic subsystem are given by
\[ \Delta H_{i+1/2,j,k}^n = D_k \Delta H_{i+1/2,j,k}^n, \quad \Delta H_{i,j+1/2,k}^n = D_k \Delta H_{i,j+1/2,k}^n, \]  

(4.49)

where \( \Delta H_{i+1/2,j}^n = H_{i+1,j}^n - H_{i,j}^n \), \( \Delta H_{i,j+1/2}^n = H_{i,j+1}^n - H_{i,j}^n \), \( D_k \) is a diagonal matrix for which the elements of the diagonal are \( (\delta_{1k}, \ldots, \delta_{kk}, \ldots, \delta_{N_D k}) \), and \( \delta \) is the usual Kronecker delta function.

### 4.4.2 Flux Limiters

The flux limiters \( \phi_{i+1/2,j,k}^n \), \( \phi_{i,j+1/2,k}^n \), \( \psi_{i+1/2,j,k}^n \), and \( \psi_{i,j+1/2,k}^n \) of Eqs. (4.19)–(4.22) are defined to be functions of the local antidiffusive flux ratios and the local CFL numbers. For the \( \zeta \)-sweep operators, \( \phi_{i+1/2,j,k}^n \) and \( \psi_{i+1/2,j,k}^n \) are determined by

\[
\phi_{i+1/2,j,k}^n = \sigma_{i+1/2,j,k}^+ \varphi_k \left( \frac{b_{i+1/2,j,k}^n}{1 + \frac{1}{2} b_{i+1/2,j,k}^n} \right) + \sigma_{i+1/2,j,k}^- \varphi_k \left( \frac{1}{1 + \frac{1}{2} b_{i+1/2,j,k}^n} \right),
\]

(4.50)

\[
\psi_{i+1/2,j,k}^n = \tilde{\sigma}_{i+1/2,j,k}^+ \varphi_k \left( \frac{\tilde{b}_{i+1/2,j,k}^n}{1 + \frac{1}{2} \tilde{b}_{i+1/2,j,k}^n} \right) + \tilde{\sigma}_{i+1/2,j,k}^- \varphi_k \left( \frac{1}{1 + \frac{1}{2} \tilde{b}_{i+1/2,j,k}^n} \right),
\]

(4.51)

where \( \varphi_k = \varphi_k(b) \) is the flux limiter function for the \( k \)-th characteristic field, \( \sigma_{i+1/2,j,k}^\pm = (\lambda_{i+1/2,j,k}^n \pm 1)/2 \), and \( \sigma_{i+1/2,j,k}^\pm \) is the sign of \( \lambda_{i+1/2,j,k}^n \) and equal to +1 if \( \lambda_{i+1/2,j,k}^n \) is positive and -1 otherwise. Equivalently, \( \tilde{\sigma}_{i+1/2,j,k}^\pm = (\tilde{\lambda}_{i+1/2,j,k}^n \pm 1)/2 \), and \( \tilde{\sigma}_{i+1/2,j,k}^\pm \) is the sign of \( \omega_{i+1/2,j}^n \). The flux ratios \( b_{i+1/2,j,k}^n \) and \( \tilde{b}_{i+1/2,j,k}^n \) for the gas-dynamic and thermodynamic subsystems are defined by the ratio of the antidiffusive fluxes

\[
b_{i+1/2,j,k}^n = \frac{\left| \lambda_{i-1/2,j,k}^n \right| - \left| \lambda_{i+1/2,j,k}^n \right|}{\Delta W_{i+1/2,j,k}^n \cdot N_{W_k}},
\]

(4.52)

\[
\tilde{b}_{i+1/2,j,k}^n = \frac{\left| \omega_{i-1/2,j}^n \right| - \left| \omega_{i+1/2,j}^n \right|}{\Delta H_{i+1/2,j,k}^n \cdot N_{H_k}},
\]

(4.53)

where \( N_{W_k} \) and \( N_{H_k} \) are normalization row vectors. In the present algorithm, \( N_{W_k} = [1, 0, 0, 0, 0, 0, 0] \) for \( k = 1, 2, \) and \( 7 \), and \( N_{W_3} = [0, 0, 0, 1, 0, 0, 0], N_{W_4} = [0, 0, 0, 0, 1, 0, 0], N_{W_5} = [0, 0, 0, 0, 0, 1, 0], \) and \( N_{W_6} = [0, 0, 0, 0, 0, 0, 1] \), and \( N_{H_k} \) is chosen to recover the component of the antidiffusive flux vector associated with the \( k \)-th component of the solution vector \( Q \). Following Sweby [1984], various combinations of flux limiter functions \( \varphi_k \) are used for each of the characteristic fields. Three different functions are employed in the present algorithm. They are the well-known \textit{minmod} limiter, van Leer's flux limiter, and the \textit{superbee} limiter of Roe given by

\[
\varphi_k(b) = \max(0, \min(1, b)),
\]

(4.54)

\[
\varphi_k(b) = \max \left( 0, \frac{2b}{1 + b} \right),
\]

(4.55)

\[
\varphi_k(b) = \max(0, \min(1, 2b), \min(2, b)),
\]

(4.56)

respectively. The latter more compressive limiter improves the sharpness of contact surfaces and slip streams. Similar formulations are used for \( \phi_{i,j+1/2,k}^n \) and \( \psi_{i,j+1/2,k}^n \) in terms of \( b_{i,j+1/2,k}^n, \tilde{b}_{i,j+1/2,k}^n, \nu_{i,j+1/2,k}^n, \) and \( \omega_{i,j+1/2,k}^n \).
4.4.3 Stability Criterion: CFL Condition

The complete semi-implicit time-marching procedure represented by Eq. (4.18) is conditionally stable. The CFL criterion

$$\Delta t^n < \min_{i,j} \left( \frac{J \Delta \zeta}{|U| + a \sqrt{x^2_i + y^2_i}}, \frac{J \Delta \eta}{|V| + a \sqrt{x^2_i + y^2_i}} \right),$$  

(4.57)

is used to restrict the magnitude of the time increment and thereby ensure stability and convergence of the numerical solution for $\Theta \geq 1/2$. In Eq. (4.57), $C_{cfl}$ is a positive valued constant in the range $0 < C_{cfl} < 1$.

4.4.4 Entropy or Wavespeed Corrections

For the most part, the TVD properties and shock resolution capabilities of Roe’s method ensure that the numerical solution furnished by the preceding semi-implicit scheme are physically realistic, nonoscillatory, and of high quality (i.e., relatively sharp and thin transitions through discontinuities and shock fronts are achieved). However, in a few situations, non-monotone behaviour can be observed and/or aphysical solutions violating entropy considerations are sometimes predicted. Even the dissipation of the fully limited first-order scheme is insufficient to damp out inaccuracies under these circumstances. In particular, four specific cases can be identified.

Expansion Shocks at Sonic Points

It is now quite well established that FDS difference solution schemes for nonlinear hyperbolic conservation laws that make use of unmodified Roe-type linearized approximate Riemann solvers are not in every instance entropy satisfying [Harten, 1983; Roe and Pike, 1984; Sweby and Baines, 1984; Chakravarthy and Osher, 1985a; Chakravarthy, 1987]. Without appropriate entropy corrections or fluxes, these schemes permit the formation of stable expansion shocks near sonic points and converge to aphysical solutions. Note that even FDS schemes based on exact Riemann solvers can exhibit small solution anomalies or glitches at sonic points [Chakravarthy and Osher, 1985a; Chakravarthy, 1987]. Refer to Figure 4.1 for an example.

This form of entropy violation is directly related to the disappearance of the inherent stabilizing numerical diffusion of the schemes as the elemental wave speeds $\lambda_k$ of the genuinely nonlinear characteristic fields approach zero. In the case of the proposed TVD schemes, this can best be understood mathematically as follows. From a consideration of the approximate Riemann solvers of Appendix A, it is easy to show that the first-order upwind numerical approximation to the $\zeta$-direction flux vector $\hat{F}$ of the gas-dynamic subsystem evaluated at the cell interface between nodes $(i, j)$ and $(i+1, j)$ can be written as

$$\hat{F}_{i+1/2,j} = \frac{1}{2} \left( \hat{F}_{i+1,j} + \hat{F}_{i,j} \right) + \frac{1}{2} \sum_{k=1}^{7} |\lambda_{i+1/2,j,k}| a_{i+1/2,j,k} e_{i+1/2,j,k},$$  

(4.58)

where the interface flux $\hat{F}_{i+1/2,j}$ has been expressed as the sum of two terms. The first term

\[\text{2It can be shown that the use of exact Riemann solutions in Godunov’s first-order upwind method provides the minimum dissipation required to prevent the formation of expansion shocks.}\]}
is the second-order arithmetic average of the flux evaluated at node points \((i, j)\) and \((i+1, j)\). This is the interface flux that would result from the application of a second-order central-difference method. The second term, containing the summation over all elemental waves, is an additional diffusive or dissipative term that acts like explicit artificial or numerical viscosity and provides the first-order upwind result. Near sonic points \(\lambda_{i+1/2,j,1} \to 0\) or \(\lambda_{i+1/2,j,7} \to 0\), as the case may be, and the diffusive term vanishes. Hence, for the particular characteristic wave, the upwind scheme reverts to the dispersive centered-difference method for which there is no numerical viscosity to prevent the generation of entropy-violating solutions.

From a physical perspective, the formation of expansion shocks can be interpreted as being related to the linearized representation of expansion waves by the approximate Riemann solver. A nonstationary one-dimensional centered rarefaction wave is a fan of characteristics across which the solution transition is continuous. Its propagation can be characterized by the leading and trailing characteristics (head and tail) of the fan. In the approximate Riemann solutions, a rarefaction wave is represented by a single discrete wave with a discontinuous solution jump. The approximate rarefaction wave possesses a single speed and direction of propagation, which may be taken to be representative of an average propagation velocity for the wave. Herein lies the difficulty. At sonic points, the leading and trailing characteristics of rarefaction waves propagate in opposite directions and thus the solution changes associated with the waves are propagated in both directions. These features cannot be represented by a single wave and velocity.

**Oscillations Behind Slow-Moving Shocks**

Aside from the difficulties at sonic points, recent research has identified other situations in which explicit and implicit FDS schemes with interface fluxes derived from linearized Riemann solutions encounter problems. Roberts [Roberts, 1990; Lin, 1991] has shown that, when solving nonlinear systems of equations in one space dimension, long wavelength numerical oscillations persist behind slow-moving (almost stationary) shock waves which are not effectively damped by the inherent diffusivity of upwind methods and additional (explicit) numerical dissipation is required to eliminate these oscillations. See Figure 4.2. Note that shock propagation for the scalar equations is well behaved. Roberts suggests a mechanism for the oscillations and shows that FDS schemes based on exact solvers also exhibit this behaviour.

**Occurrence of Negative Densities and Internal Energies**

In other work relating to the application of Godunov-type schemes for the solution of the Euler equations, the recent analysis of Einfeldt *et al.* [1991] has demonstrated that schemes employing approximate Riemann solvers of the type used in the proposed semi-implicit TVD scheme are not *positively conservative*, in other words, the computed density and internal energy are not guaranteed to remain greater than zero which, of course, is physically unrealistic. They prove that for some initial data involving strong rarefaction waves or strong shear flows, Roe-type linearized Riemann solvers will produce vacuum states with negative values of density and/or pressure even though the various state pressures and densities of the exact solution are all positive. An example of this is illustrated in Figure 4.3. Ensuring that solutions schemes are positively conservative is obviously of considerable importance, particularly for high-speed hypersonic flow studies, where densities are low.
and most of the flow energy is in the form of kinetic energy.

**Carbuncle Phenomenon for Blunt-Body Flows**

Although not discussed extensively in the literature, it also appears to be quite well known that the use of approximate and exact Riemann solvers to compute supersonic (or hypersonic) flow over two-dimensional blunt bodies can lead to numerical instabilities [Lin, 1991; Yee et al., 1990]. During the numerical computation of such flows via a time-marching FDS approach, a numerical instability may form as the bow shock approaches its steady-state position. This instability has been termed the carbuncle phenomenon by researchers at NASA [Lin, 1991]. In some cases, the instability causes the numerical solution to deteriorate completely, as depicted in Figure 4.4, whereas, in other cases, the only evidence of the instability are numerical oscillations which degrade the solution in the subsonic region behind the bow shock. In either case, the carbuncle phenomenon is undesirable. The causes of the carbuncle instability are not fully understood; however, it is felt that it may be related to the numerical oscillations associated with slow-moving shocks discussed above.

**Proposed Wavespeed Corrections**

It is possible to modify Roe's method to alleviate the inaccuracies associated with each of the preceding situations and a number of correction procedures have been proposed. Various entropy or sonic-point corrections are offered by Harten [1983], Roe and Pike [1984], Chakravarthy and Osher [1985a], and Dubois and Mehlman [1991], and remedies for the oscillations associated with slow-moving shocks and the blunt-body carbuncle phenomenon have been devised by Yee et al. [1990] and Lin [1991]. In addition, the analysis of Einfeldt et al. [1991] provides an entropy fix that results in positively conservative schemes. Many of the techniques are, to some extent, ad hoc and, in virtually all of these proposals, additional explicit or artificial dissipation is added to the dissipation already present in the underlying first-order method by modifying the wave speeds that result from the approximate Riemann solver. Hence, the term wave speed correction is often used.

For the proposed semi-implicit method, a variant of the entropy fix suggested by Roe and Pike [1984] is employed herein which modifies the scheme near sonic points and thereby makes certain that the method is entropy satisfying and converges to the correct physical solution. In particular, the flux functions associated with nonlinear characteristic fields 1 and 7 of the spatial operators \( \mathcal{L}_{W_i}^{n} \) and \( \mathcal{L}_{W_i}^{n+1} \) must be augmented to prevent the formation of aphysical expansion shocks. Consider elemental wave 1 of the operator \( \mathcal{L}_{W_i}^{n+1} \). A wave spreading parameter for this wave is defined to be

\[
\delta_{i+1/2,j,1}^n = 2 \left[ \lambda_{i+1/2,j,1}^n - \left( \frac{U_{i,j}^n - a_{i,j}^n \sqrt{x_{i+1/2,j,1}^2 + y_{i+1/2,j,1}^2}}{\Delta w_{i+1/2,j,1}^n} \right) \right]. \tag{4.59}
\]

If \( \lambda_{i+1/2,j,1}^n - 1/2\delta_{i+1/2,j,1}^n < 0 \) and \( \lambda_{i+1/2,j,1}^n + 1/2\delta_{i+1/2,j,1}^n > 0 \), then the flux limiter \( \phi_{i+1/2,j,1}^n \) is set to zero and the first-order flux jump is split into two components, that is,

\[
\frac{1}{2} \left( \nu_{i+1/2,j,1}^n - |\nu_{i+1/2,j,1}^n| \right) \Delta W_{i+1/2,j,1}^n, \tag{4.60}
\]
is replaced by
\[
\frac{1}{2}(\nu_{i+1/2,j,1}^{n+} - |\nu_{i+1/2,j,1}^{n+}|)\Delta W_{i+1/2,j,1}^n + \frac{1}{2}(\nu_{i+1/2,j,1}^{n-} - |\nu_{i+1/2,j,1}^{n-}|)\Delta W_{i+1/2,j,1}^n,
\]
(4.61)
where
\[
\nu_{i+1/2,j,1}^{n+} = (\lambda_{i+1/2,j,1}^n + \frac{1}{2}\delta_{i+1/2,j,1}^n), \quad \nu_{i+1/2,j,1}^{n-} = (\lambda_{i+1/2,j,1}^n - \frac{1}{2}\delta_{i+1/2,j,1}^n).
\]
(4.62)

Equivalent procedures are required for the other three nonlinear characteristic fields.

Although the preceding entropy correction does not guarantee that the solution algorithm is positively conservative, it is generally sufficient for most unsteady flow applications. A more sophisticated wave speed correction procedure is utilized in the fully implicit technique for stationary flow problems of the next section.

### 4.4.5 Preservation of Positivity and Maximum Principles

Aside from concerns that the proposed difference scheme satisfy entropy conditions and preserve the positivity of the density, it also desirable that the method preserve the positivity of and maximum principle for the mass fractions of each species $c_s$ as defined by Larrouturou [1991]. This guarantees that $0 \leq c_s \leq 1$ and $\sum_s c_s = 1$. The consequences of not satisfying these conditions are undesirable. It was stated in the description of the equation decoupling procedure that the approximate solutions of proposed TVD schemes preserve discrete forms of the positivity and the maximum principles for the mass fractions. A partial proof of this is now given under a set of restrictive conditions.

Before proceeding with the argument, some definitions are necessary. Discrete solution schemes for the Euler equations of Eqs. (3.8)-(3.10) that preserve the positivity of the mass fractions can be defined as follows:

**Definition 4.1** Fully discrete solution schemes for the Euler equations of thermochemical nonequilibrium flow (Eqs. (3.8)-(3.10), $w_s \neq 0$) preserve the positivity of the mass fraction $c_{s_{i,j}}^n$ if, for all $i$ and $j$ and $n \geq 0$,

\[
c_{s_{i,j}}^n \geq 0.
\]
(4.63)

Moreover, Larrouturou [1991] defines the maximum principles for the mass fractions for discrete solutions in the nonreacting and reacting flow cases as follows:

**Definition 4.2 (Larrouturou)** Fully discrete solution schemes for the Euler equations of nonreacting thermal nonequilibrium flow (Eqs. (3.8)-(3.10), with $w_s = 0$) preserve the maximum principle for the mass fraction $c_{s_{i,j}}^n$ if, for all $i$ and $j$ and $n \geq 0$,

\[
\min_{i,j} c_{s_{i,j}}^0 \leq c_{s_{i,j}}^n \leq \max_{i,j} c_{s_{i,j}}^0.
\]
(4.64)

4.17
Definition 4.3 (Larrouturou) Fully discrete solution schemes for the Euler equations of thermochemical nonequilibrium flow (Eqs. (3.8)-(3.10), \( w_s \neq 0 \)) preserve the maximum principle for the mass fraction \( c_{s,i,j}^n \) if, for all \( i \) and \( j \) and \( n \geq 0 \),

\[
0 \leq c_{s,i,j}^n \leq \max_{i,j} c_{s,i,j}^0, \quad \text{if} \quad \min_{i,j} c_{s,i,j}^0 \geq 0.
\]

(4.65)

Note that these definitions imply that if a solution scheme preserves the maximum principle, it is also positively conservative in terms of the mass fractions.

For the purposes of the proof, we shall consider only the first-order version (\( \phi_{i+1/2,j,k}^n = \Phi_{i+1/2,j,k} = \Psi_{i+1/2,j,k} = 0 \)) of the semi-implicit TVD scheme of Eqs. (4.18)-(4.22) with \( \Theta = 1 \). It will further be assumed, as Larrouturou has done, that the source term describing the time rate of change of the species mass fraction has the simplified form

\[
w_s = -K_s c_s^0,
\]

(4.66)

where \( K_s \) is a constant, with \( K_s > 0 \). This expression implies that the species \( s \) is being consumed at a rate that is directly proportional to its concentration. Under these conditions, the time-split scheme for the species mass concentration equations of the thermodynamic scheme can be written as

\[
c_{s,i,j}^{n+1} = L_{c_i}^{\Delta t} L_{c_j}^{\Delta t} L_{c_s}^{\Delta t} c_{s,i,j}^n,
\]

(4.67)

where the \( L_{c_i}^{\Delta t} \) and \( L_{c_j}^{\Delta t} \) solution operators are given by

\[
L_{c_i}^{\Delta t} c_{s,i,j}^n = c_{s,i,j}^{n+1}: c_{s,i,j}^{n+1} = c_{s,i,j}^n - \frac{1}{2} (\omega_{i+1/2,j}^n - |\omega_{i+1/2,j}^n|) (c_{s,i+1,j}^n - c_{s,i,j}^n) - \frac{1}{2} (\omega_{i-1/2,j}^n + |\omega_{i-1/2,j}^n|) (c_{s,i,j}^n - c_{s,i-1,j}^n) - \Delta t K_s c_{s,i,j}^{n+1},
\]

(4.68)

\[
L_{c_j}^{\Delta t} c_{s,i,j}^n = c_{s,i,j}^{n+1}: c_{s,i,j}^{n+1} = c_{s,i,j}^n - \frac{1}{2} (\omega_{i,j+1/2}^n - |\omega_{i,j+1/2}^n|) (c_{s,i,j+1}^n - c_{s,i,j}^n) - \frac{1}{2} (\omega_{i,j-1/2}^n + |\omega_{i,j-1/2}^n|) (c_{s,i,j}^n - c_{s,i,j-1}^n).
\]

(4.69)

For a restricted time step \( \Delta t^n \), the time-split scheme above preserves the maximum principle of Definition 4.3.

Proposition 4.1 The time-split upwind difference scheme of Eqs. (4.67)-(4.69) preserves the maximum principle of Definition 4.3 for the mass fraction \( c_{s,i,j}^n \) under the CFL-like conditions

\[
|\omega_{i+1/2,j}^n| \leq \frac{1}{2}, \quad |\omega_{i,j+1/2}^n| \leq \frac{1}{2},
\]

(4.70)

for all \( i \) and \( j \) and \( n \geq 0 \).
Proof. The proof of Proposition 4.1 is rather straightforward. Consider first the $L_{c^n}^{\Delta t}$ operator. Four cases must be considered. They are

(i) If $\omega_{i,j+1/2}^n < 0$ and $\omega_{i,j-1/2}^n < 0$, then the updated species concentration is

$$c_{s_{i,j}}^{n+1} = (1 - |\omega_{i,j+1/2}^n|)c_{s_{i,j}}^n + |\omega_{i,j+1/2}^n|c_{s_{i,j+1}}^n.$$  (4.71)

(ii) If $\omega_{i,j+1/2}^n > 0$ and $\omega_{i,j-1/2}^n > 0$, then the updated species concentration is

$$c_{s_{i,j}}^{n+1} = |\omega_{i-1/2,j}^n|c_{s_{i,j-1}}^n + (1 - |\omega_{i-1/2,j}^n|)c_{s_{i,j}}^n.$$  (4.72)

(iii) If $\omega_{i,j+1/2}^n > 0$ and $\omega_{i,j-1/2}^n < 0$, then the updated species concentration is

$$c_{s_{i,j}}^{n+1} = c_{s_{i,j}}^n.$$  (4.73)

(iv) If $\omega_{i,j+1/2}^n < 0$ and $\omega_{i,j-1/2}^n > 0$, then the updated species concentration is

$$c_{s_{i,j}}^{n+1} = |\omega_{i,j-1/2}^n|c_{s_{i,j-1}}^n + (1 - |\omega_{i,j+1/2}^n| - |\omega_{i,j-1/2}^n|)c_{s_{i,j}}^n + |\omega_{i,j+1/2}^n|c_{s_{i,j+1}}^n.$$  (4.74)

Observe that, in all four cases, the updated mass fraction $c_{s_{i,j}}^{n+1}$ is a linear weighted combination of $c_{s_{i,j-1}}^n$, $c_{s_{i,j}}^n$, and $c_{s_{i,j+1}}^n$, where the sum of the weighting coefficients is unity and, if $|\omega_{i,j+1/2}^n| < 1/2$ and $|\omega_{i,j-1/2}^n| < 1/2$, the coefficients are all positive. If it is further assumed that $\min c_{s_{i,j-1}}^0 \leq c_{s_{i,j}}^n \leq \max c_{s_{i,j}}^0$, then the updated mass fraction also satisfies the inequality $\min c_{s_{i,j}}^0 \leq c_{s_{i,j}}^{n+1} \leq \max c_{s_{i,j}}^0$, and hence the $L_{c^n}^{\Delta t}$ operator preserves the maximum principle in the sense of Definition 4.2.

Consider next the $L_{c_i}^{\Delta t}$ operator. Four cases must again be considered. They are

(i) If $\omega_{i+1/2,j}^n < 0$ and $\omega_{i-1/2,j}^n < 0$, then the updated species concentration is

$$c_{s_{i,j}}^{n+1} = \frac{1 - |\omega_{i+1/2,j}^n|}{1 + \Delta t^n K_s} c_{s_{i,j}}^n + \frac{|\omega_{i+1/2,j}^n|}{1 + \Delta t^n K_s} c_{s_{i,j+1}}^n.$$  (4.75)

(ii) If $\omega_{i+1/2,j}^n > 0$ and $\omega_{i-1/2,j}^n > 0$, then the updated species concentration is

$$c_{s_{i,j}}^{n+1} = \frac{|\omega_{i-1/2,j}^n|}{1 + \Delta t^n K_s} c_{s_{i,j-1}}^n + \frac{1 - |\omega_{i-1/2,j}^n|}{1 + \Delta t^n K_s} c_{s_{i,j}}^n.$$  (4.76)
(iii) If $\omega_{i+1/2,j}^n > 0$ and $\omega_{i-1/2,j}^n < 0$, then the updated species concentration is

$$c_{s_{i,j}}^{n+1} = \frac{1}{1 + \Delta t^n K_s} c_{s_{i,j}}^n,$$  \hspace{1cm} (4.77)

(iv) If $\omega_{i+1/2,j}^n < 0$ and $\omega_{i-1/2,j}^n > 0$, then the updated species concentration is

$$c_{s_{i,j}}^{n+1} = \frac{|\omega_{i-1/2,j}^n|}{1 + \Delta t^n K_s} c_{s_{i,j}}^{n-1} + \frac{1 - |\omega_{i+1/2,j}^n| - |\omega_{i-1/2,j}^n|}{1 + \Delta t^n K_s} c_{s_{i,j}}^n + \frac{|\omega_{i+1/2,j}^n|}{1 + \Delta t^n K_s} c_{s_{i,j}}^{n+1}.$$  \hspace{1cm} (4.78)

In these cases, the updated mass fraction $c_{s_{i,j}}^{n+1}$ is a linear weighted combination of $c_{s_{i,j}}^{n-1}$, $c_{s_{i,j}}^n$, and $c_{s_{i,j}}^{n+1}$, and the weighting coefficients are all positive if $|\omega_{i+1/2,j}^n| < 1/2$ and $|\omega_{i-1/2,j}^n| < 1/2$. The sum of the weighting coefficients is $1/(1 + \Delta t^n K_s)$, which is less than unity for $K_s > 0$. If $0 \leq c_{s_{i,j-1}}^n \leq \max c_s$, $0 \leq c_{s_{i,j}}^n \leq \max c_s$, and $0 \leq c_{s_{i,j+1}}^n \leq \max c_s$, then $0 \leq c_{s_{i,j}}^{n+1} \leq \max c_s$, and it is evident that the $C^{\Delta t}_{c_N}$ operator preserves the maximum principle as given by Definition 4.3. The fact that both time split operators preserve the maximum principle implies that the difference scheme of Eqs. (4.67)-(4.69) also preserves the maximum principle of Definition 4.3 and this completes the proof. Note that an appropriate choice of $C_{c_N}$ in the CFL condition of Eq. (4.57) will ensure that the inequalities $|\omega_{i+1/2,j}^n| < 1/2$ and $|\omega_{i,j+1/2}^n| < 1/2$ hold.

Having demonstrated Proposition 4.1, it remains to be shown that the first-order version of the semi-implicit scheme satisfies the maximum principle for $N$ species, with $N \geq 2$, and $\sum_s c_s = 1$. If the first-order scheme is applied to the mass fraction equations for species $s = 1, 2, \ldots, N-1$ and the mass fraction $c_N$ is evaluated as $c_N = 1 - \sum_{s=1}^{N-1} c_s$, then it is assured that $\sum_s c_s = 1$ and $0 \leq c_s \leq 1$ for $s = 1, 2, \ldots, N-1$. Moreover, it can be shown that $0 \leq c_N \leq 1$. This can be seen as follows. For the $C^{\Delta t}_{c_N}$ operator with $\omega_{i,j+1/2}^n < 0$ and $\omega_{i,j-1/2}^n > 0$, $c_N = 1 - \sum_{s=1}^{N-1} c_s$ can be rewritten as

$$c_{N_{i,j}}^{n+1} = 1 - |\omega_{i,j+1/2}^n| \sum_{s=1}^{N-1} c_{s_{i,j-1}}^n - (1 - |\omega_{i,j+1/2}^n| - |\omega_{i,j-1/2}^n|) \sum_{s=1}^{N-1} c_{s_{i,j}}^n - |\omega_{i,j+1/2}^n| \sum_{s=1}^{N-1} c_{s_{i,j+1}}^n.$$  \hspace{1cm} (4.79)

Noting that $\sum_{s=1}^{N-1} c_{s_{i,j-1}}^n = 1 - c_{N_{i,j-1}}$, $\sum_{s=1}^{N-1} c_{s_{i,j}}^n = 1 - c_{N_{i,j}}$, and $\sum_{s=1}^{N-1} c_{s_{i,j+1}}^n = 1 - c_{N_{i,j+1}}$, the equation can be rewritten and re-expressed as

$$c_{N_{i,j}}^{n+1} = |\omega_{i,j-1/2}^n| c_{N_{i,j-1}} + (1 - |\omega_{i,j+1/2}^n| - |\omega_{i,j-1/2}^n|) c_{N_{i,j}} + |\omega_{i,j+1/2}^n| c_{N_{i,j+1}}.$$  \hspace{1cm} (4.80)

which is a weighted sum of the form described above. Hence, the maximum principle for $c_N$ is satisfied. Similar results apply for the other three combinations of signs of $\omega_{i,j+1/2}^n$ and $\omega_{i,j-1/2}^n$. 

4.20
For the $L_c^{At}$ operator with $\omega_{i+1/2,j}^n < 0$ and $\omega_{i-1/2,j}^n > 0$, it can be shown that

$$c_{Ni,J}^{n+1} = 1 - \frac{\left|\omega_{i-1/2,j}^n\right|}{1 + \Delta t^n K_s} \sum_{s=1}^{N-1} c_{Ni-1,s}^n - \frac{1 - \left|\omega_{i+1/2,j}^n\right| - \left|\omega_{i-1/2,j}^n\right|}{1 + \Delta t^n K_s} \sum_{s=1}^{N-1} c_{Ni,s}^n$$

$$+ \left(\frac{\Delta t^n K_s}{1 + \Delta t^n K_s}\right) c_{Ni-1,j}^n + \frac{\left|\omega_{i+1/2,j}^n\right|}{1 + \Delta t^n K_s} c_{Ni+1,j}^n - \frac{\left|\omega_{i-1/2,j}^n\right|}{1 + \Delta t^n K_s} c_{Ni,j}^n$$

Which can be rewritten as

$$c_{Ni,J}^{n+1} = \frac{\Delta t^n K_s}{1 + \Delta t^n K_s} + \frac{\left|\omega_{i-1/2,j}^n\right|}{1 + \Delta t^n K_s} c_{Ni-1,j}^n$$

$$+ \frac{1 - \left|\omega_{i+1/2,j}^n\right| - \left|\omega_{i-1/2,j}^n\right|}{1 + \Delta t^n K_s} c_{Ni,s}^n + \frac{\left|\omega_{i+1/2,j}^n\right|}{1 + \Delta t^n K_s} c_{Ni+1,j}^n$$

This is also a weighted sum of the form described above and therefore, the maximum principle for $c_N$ is again satisfied. Similar results follow for the other three combinations of signs of $\omega_{i+1/2,j}^n$ and $\omega_{i-1/2,j}^n$.

Thus, it has been shown that the first-order version of the partially-decoupled semi-implicit TVD scheme with source terms $w_s = -K_s c_s$ satisfies the positivity and maximum principles for the mass fraction $c_s$ in the case of a mixture of $N$ species. On the basis of this result and some others offered by Larrouturou [1991], it is possible to argue that the higher-order scheme of this section and the fully implicit schemes, to be described in the next section, also preserve the positivity of and maximum principles for the mass fractions. Note that Larrouturou points out that chemistry-split and FDS fully coupled solution schemes do not always satisfy these important principles.

### 4.4.6 Effects of Increasing Stiffness

For very stiff cases, the time step imposed by Eq. (4.57) can be much larger than the fastest times scales associated with the finite-rate source terms. Although the present semi-implicit algorithm should remain stable, this may result in the loss of accuracy in predicted nonequilibrium shock-front structure. For many applications, this form of solution degradation is not too detrimental as the computed jump conditions and propagation speeds of the discontinuities should still be physically correct, provided that the spatial resolution of the grid is sufficient. If more accurate resolution of relaxation fronts is required, then smaller time increments will improve the situation; however, it should be emphasized that spatial resolution is as important as temporal resolution. LeVeque and Yee [1990] and Griffiths et al. [1992] have studied the construction of numerical solutions for model scalar advection equations with nonlinear source terms. Both fully coupled and split solution algorithms were considered. For very stiff problems, they have shown that in some cases the schemes produce incorrect propagation speeds for discontinuities and that these wave propagation errors result from a lack of spatial resolution. In particular, Griffiths et al. have contrasted coupled explicit monotone and (chemistry) split schemes and have shown that, with increasing stiffness, the solutions of the split schemes remain monotone and
bounded but the predicted or numerical propagation speeds do not coincide with the actual or true wave speeds. They have also shown that the coupled schemes diverge with increasing stiffness. Numerical computations of one-dimensional shock wave propagation problems in air were performed as part of the present study (refer to Chapter 6) using the proposed partially-decoupled semi-implicit method. Although the results confirm to some extent the observations of LeVeque and Yee and Griffiths et al. and indicate that care must be exercised in selecting the spatial mesh to ensure that discontinuities are sufficiently resolved, in general it was found that the predictions were satisfactory. It is felt that further study of these effects of stiffness is warranted.

4.5 Factored Fully Implicit TVD Scheme

The preceding semi-implicit scheme is not very appropriate for computing steady-state solutions to the thermochemical nonequilibrium Euler equations. Moreover, fully implicit extensions of the method are not straightforward because the underlying scalar scheme is such that the spatial and time discretization procedures are coupled. Therefore, a factored fully implicit scheme is also proposed, based on an alternative TVD upwind formulation, for the solution of Eq. (3.8) via the partially-decoupled approach and the time integration of Eqs. (4.1) and (4.3). This scheme is more suitable for steady-state applications.

The basic solution approach follows those given by Chakravarthy [1987] for perfect gases. The numerical flux functions of both the gas-dynamic and thermodynamic subsystems are evaluated by applying the flux-difference splitting technique used in the preceding semi-implicit scheme in conjunction with the one-parameter family of semi-discrete higher-order TVD upwind methods devised by Osher and Chakravarthy [Osher and Chakravarthy, 1984; Chakravarthy and Osher, 1985b; Chakravarthy and Osher, 1985a] as the underlying scalar schemes. The spatial discretization is coupled to a two-step two-parameter implicit time discretization. A factored nonconservative linearization procedure is employed for the implicit operators in which only the first-order terms of the spatial discretization are considered and the Roe-average state, eigenvalues, and eigenvectors of the flux Jacobians are assumed to be slowly varying functions of the solution vectors and are thus treated as locally constant. The factorization of the implicit operators avoids the inversion of very large matrices. The first-order linearization technique has the disadvantage that time accuracy is essentially lost because the implicit operators are not conservative and the implicit and explicit operators no longer possess the same spatial accuracy. However, the underlying scheme can be shown to be TVD and has the advantage that it is simple and efficient to implement. Additionally, by including the higher-order terms in the explicit operators, steady-state solutions will possess the high-accuracy features and required conservation properties. Similar implicit linearization procedures have been used elsewhere (e.g., Mulder and van Leer [1985]).

4.5.1 Discretized Equations

The two-parameter partially-decoupled factored fully implicit scheme can be expressed as

$$U_{i,j}^{n+1} = \mathcal{L}_W^{\Delta t} \mathcal{L}_Q^{\Delta t} U_{i,j}^n,$$

where $\mathcal{L}_W^{\Delta t} U_{i,j} = U(W_{i,j}^{n+1}, Q_{i,j}^n)$ and the fully discrete gas-dynamic solution operator $\mathcal{L}_W^{\Delta t}$ is
\[
\begin{align*}
&\left[ \frac{\Theta}{1 + \Omega} \sum_{k=1}^{7} \left( \nu_{i,j+1/2,k}^{n} e_{i,j+1/2,k}^{n} A_{i,j+1/2,k}^{-n} \right) \right] \Delta W_{i,j+1}^{n} \\
&+ \left[ I + \frac{\Theta}{1 + \Omega} \sum_{k=1}^{7} \left( \nu_{i,j+1/2,k}^{-n} e_{i,j+1/2,k}^{n} B_{i,j+1/2,k}^{-n} + \nu_{i,j-1/2,k}^{+n} e_{i,j-1/2,k}^{n} B_{i,j-1/2,k}^{+n} \right) \right] \Delta W_{i,j}^{n} \\
&+ \left[ \frac{\Theta}{1 + \Omega} \sum_{k=1}^{7} \left( \nu_{i,j-1/2,k}^{+n} e_{i,j-1/2,k}^{n} C_{i,j-1/2,k}^{+n} \right) \right] \Delta W_{i,j-1}^{n}
\end{align*}
\]
\[
\frac{\Omega}{1 + \Omega} \Delta W_{i,j}^{n-1} - \frac{1}{1 + \Omega} \sum_{k=1}^{7} \left[ \nu_{i+1/2,j,k}^{-n} \Delta W_{i+1/2,j,k}^{n} \right]
+ \nu_{i+1/2,j,k}^{+n} \Delta W_{i+1/2,j,k}^{n} + \nu_{i,j+1/2,k}^{-n} \Delta W_{i,j+1/2,k}^{n}
+ \nu_{i,j-1/2,k}^{+n} \Delta W_{i,j-1/2,k}^{n} + \nu_{i,j-1/2,k}^{-n} \Delta W_{i,j-1/2,k}^{n}
+ \frac{1}{4} \left( \phi_{i+1/2,j,k}^{-n} v_{i+1/2,j,k}^{-n} \Delta W_{i+1/2,j,k}^{n} - \phi_{i+1/2,j,k}^{+n} v_{i+1/2,j,k}^{+n} \Delta W_{i+1/2,j,k}^{n} \right)
+ \frac{1}{4} \left( \phi_{i,j+1/2,k}^{-n} v_{i,j+1/2,k}^{-n} \Delta W_{i,j+1/2,k}^{n} - \phi_{i,j+1/2,k}^{+n} v_{i,j+1/2,k}^{+n} \Delta W_{i,j+1/2,k}^{n} \right)
+ \frac{1}{4} \left( \phi_{i,j-1/2,k}^{-n} v_{i,j-1/2,k}^{-n} \Delta W_{i,j-1/2,k}^{n} - \phi_{i,j-1/2,k}^{+n} v_{i,j-1/2,k}^{+n} \Delta W_{i,j-1/2,k}^{n} \right)
+ \frac{1}{4} \left( \phi_{i,j}^{-n} v_{i,j}^{-n} \Delta W_{i,j}^{n} - \phi_{i,j}^{+n} v_{i,j}^{+n} \Delta W_{i,j}^{n} \right)
+ \frac{1}{4} \left( \phi_{i,j}^{-n} v_{i,j}^{-n} \Delta W_{i,j}^{n} - \phi_{i,j}^{+n} v_{i,j}^{+n} \Delta W_{i,j}^{n} \right)
+ \frac{1}{4} \left( \phi_{i,j}^{-n} v_{i,j}^{-n} \Delta W_{i,j}^{n} - \phi_{i,j}^{+n} v_{i,j}^{+n} \Delta W_{i,j}^{n} \right)
+ \frac{1}{4} \left( \phi_{i,j}^{-n} v_{i,j}^{-n} \Delta W_{i,j}^{n} - \phi_{i,j}^{+n} v_{i,j}^{+n} \Delta W_{i,j}^{n} \right)
\] 
(4.84)
\[
\begin{align*}
&\left[ \frac{\Theta}{1 + \Omega} \sum_{k=1}^{7} \left( \nu_{i+1/2,j,k}^{-n} e_{i+1/2,j,k}^{n} A_{i+1/2,j,k}^{-n} \right) \right] \Delta W_{i+1,j}^{n} \\
&+ \left[ I + \frac{\Theta}{1 + \Omega} \sum_{k=1}^{7} \left( \nu_{i+1/2,j,k}^{-n} e_{i+1/2,j,k}^{n} B_{i+1/2,j,k}^{-n} + \nu_{i,j+1/2,k}^{+n} e_{i,j+1/2,k}^{n} B_{i,j+1/2,k}^{+n} \right) \right] \Delta W_{i,j}^{n} \\
&+ \left[ \frac{\Theta}{1 + \Omega} \sum_{k=1}^{7} \left( \nu_{i,j-1/2,k}^{+n} e_{i,j-1/2,k}^{n} C_{i,j-1/2,k}^{+n} \right) \right] \Delta W_{i,j-1}^{n} = \Delta W_{i,j}^{n},
\end{align*}
\] 
(4.85)
\[
\Delta W_{i,j}^{n} = W_{i,j}^{n} + \Delta W_{i,j}^{n},
\] 
(4.86)
\[
\text{and where } \mathcal{L}_{\Omega}^{\Delta t} U_{i,j}^{n} = U(W_{i,j}^{n}, Q_{i,j}^{n+1}) \text{ and the thermodynamic solution operator } \mathcal{L}_{\Omega}^{\Delta t} \text{ is}
\]

4.23
\[
\begin{align*}
\frac{\theta}{1 + \Omega} \omega_{i+1/2,j}^n D_N \Delta Q_{i,j}^n &+ \left[ I - \frac{\theta}{1 + \Omega} (\omega_{i+1/2,j}^n - \omega_{i-1/2,j}^n) D_N \right] \Delta Q_{i,j}^n - \frac{\theta}{1 + \Omega} \omega_{i,j-1/2}^n D_N \Delta Q_{i,j-1}^n = \\
\frac{\Omega}{1 + \Omega} \Delta Q_{i,j}^{n-1} + \Delta t^n \Delta S_{i,j}^n - \frac{1}{1 + \Omega} \sum_{k=1}^{2N+1} \left[ \omega_{i+1/2,j}^n \Delta H_{i+1/2,j,k}^n \right] \\
+ \omega_i^{+ n} \Delta H_{i-1/2,j,k}^n + \omega_{i,j+1/2}^{- n} \Delta H_{i,j+1/2,k}^n + \omega_{i,j-1/2}^{- n} \Delta H_{i,j-1/2,k}^n \\
+ \frac{1}{4} \left( \psi_{i+1/2,j,k}^{+ n} \omega_{i+1/2,j,k}^{- n} \Delta H_{i+1/2,j,k}^n - \psi_{i+1/2,j,k}^{- n} \omega_{i+1/2,j,k}^{+ n} \Delta H_{i+1/2,j,k}^n \right) \\
+ \frac{1}{4} \left( \tilde{\psi}_{i+1/2,j,k}^{- n} \omega_{i+1/2,j,k}^{+ n} \Delta H_{i+1/2,j,k}^n - \tilde{\psi}_{i+1/2,j,k}^{+ n} \omega_{i+1/2,j,k}^{- n} \Delta H_{i+1/2,j,k}^n \right) \\
+ \frac{1}{4} \left( \psi_{i-1/2,j,k}^{+ n} \omega_{i-1/2,j,k}^{- n} \Delta H_{i-1/2,j,k}^n - \psi_{i-1/2,j,k}^{- n} \omega_{i-1/2,j,k}^{+ n} \Delta H_{i-1/2,j,k}^n \right) \\
+ \frac{1}{4} \left( \tilde{\psi}_{i-1/2,j,k}^{- n} \omega_{i-1/2,j,k}^{+ n} \Delta H_{i-1/2,j,k}^n - \tilde{\psi}_{i-1/2,j,k}^{+ n} \omega_{i-1/2,j,k}^{- n} \Delta H_{i-1/2,j,k}^n \right) \\
+ \frac{1}{4} \left( \psi_{i,j+1/2,k}^{+ n} \omega_{i,j+1/2,k}^{- n} \Delta H_{i,j+1/2,k}^n - \psi_{i,j+1/2,k}^{- n} \omega_{i,j+1/2,k}^{+ n} \Delta H_{i,j+1/2,k}^n \right) \\
+ \frac{1}{4} \left( \tilde{\psi}_{i,j+1/2,k}^{- n} \omega_{i,j+1/2,k}^{+ n} \Delta H_{i,j+1/2,k}^n - \tilde{\psi}_{i,j+1/2,k}^{+ n} \omega_{i,j+1/2,k}^{- n} \Delta H_{i,j+1/2,k}^n \right) \\
+ \frac{1}{4} \left( \psi_{i,j-1/2,k}^{+ n} \omega_{i,j-1/2,k}^{- n} \Delta H_{i,j-1/2,k}^n - \psi_{i,j-1/2,k}^{- n} \omega_{i,j-1/2,k}^{+ n} \Delta H_{i,j-1/2,k}^n \right) \\
+ \frac{1}{4} \left( \tilde{\psi}_{i,j-1/2,k}^{- n} \omega_{i,j-1/2,k}^{+ n} \Delta H_{i,j-1/2,k}^n - \tilde{\psi}_{i,j-1/2,k}^{+ n} \omega_{i,j-1/2,k}^{- n} \Delta H_{i,j-1/2,k}^n \right) \right], \quad (4.87)
\end{align*}
\]

\[
\frac{\theta}{1 + \Omega} \omega_{i+1/2,j}^n D_N \Delta Q_{i+1,j}^n + \left[ I - \frac{\theta}{1 + \Omega} (\omega_{i+1/2,j}^n - \omega_{i-1/2,j}^n) D_N \right] \Delta Q_{i+1,j}^n - \frac{\theta}{1 + \Omega} \omega_{i,j-1/2}^n D_N \Delta Q_{i,j-1}^n = \Delta Q_{i,j}^n, \quad (4.88)
\]

\[
\hat{Q}_{i,j}^n = Q_{i,j}^n + \Delta Q_{i,j}^n, \quad (4.89)
\]

and \( \Delta W_{i,j}^n \) and \( \Delta Q_{i,j}^n \) again denote intermediate solutions. Equations (4.84)–(4.89) represent block and scalar tridiagonal systems of linear equations for the solution changes which can be solved using standard techniques [Anderson et al., 1984].

The two parameters \( \Theta \) and \( \Omega \) control the temporal discretization of the two-step algorithm. For \( \Theta \neq 0 \) the partially-decoupled scheme is implicit and if \( \Theta = \Omega + 1/2 \) the time marching becomes second-order accurate. Some specific schemes can be identified. One-
step methods are obtained for $\Omega = 0$. In this case, the time differencing is Euler explicit for $\Theta = 0$, trapezoidal implicit for $\Theta = 1/2$, and Euler implicit for $\Theta = 1$. A second-order three-point backward implicit time differencing scheme is achieved for $\Theta = 1$ and $\Omega = 1/2$. Beam and Warming [1982] provide a detailed analysis of two-level linear multistep time-marching methods relevant to CFD applications.

In Eqs. (4.84)-(4.89), $\nu_{i+1/2,j,k}^{+}$, $\nu_{i+1/2,j,k}^{-}$, $\omega_{i+1/2,j}^{+}$, and $\omega_{i+1/2,j}^{-}$ are the positive and negative CFL numbers defined by

$$
\nu_{i+1/2,j,k}^{+} = \frac{1}{2}(\nu_{i+1/2,j,k}^{n} \pm |\nu_{i+1/2,j,k}^{n}| \pm \delta \nu_{i+1/2,j,k}^{n}),
$$

(4.90)

$$
\nu_{i,j+1/2,k}^{+} = \frac{1}{2}(\nu_{i,j+1/2,k}^{n} \pm |\nu_{i,j+1/2,k}^{n}| \pm \delta \nu_{i,j+1/2,k}^{n}),
$$

(4.91)

$$
\omega_{i+1/2,j}^{+} = \frac{1}{2}(\omega_{i+1/2,j}^{n} \pm |\omega_{i+1/2,j}^{n}| \pm \delta \omega_{i+1/2,j}^{n}),
$$

(4.92)

$$
\omega_{i+1/2,j}^{-} = \frac{1}{2}(\omega_{i+1/2,j}^{n} \pm |\omega_{i+1/2,j}^{n}| \pm \delta \omega_{i+1/2,j}^{n}),
$$

(4.93)

for which $\delta \nu$ and $\delta \omega$ are wave speed corrections that ensure that solutions are entropy satisfying. $A_{i+1/2,j,k}^{-}$, $B_{i+1/2,j,k}^{+}$, and $C_{i-1/2,j,k}^{+}$ are seven-component column vectors defined by

$$
A_{i+1/2,j,k}^{-} = \frac{\partial \alpha_{i+1/2,j,k}^{n}}{\partial W_{i+1,j}^{n}}, \quad B_{i+1/2,j,k}^{+} = \frac{\partial \alpha_{i\pm1/2,j,k}^{n}}{\partial W_{i,j}^{n}}, \quad C_{i-1/2,j,k}^{+} = \frac{\partial \alpha_{i-1/2,j,k}^{n}}{\partial W_{i-1,j}^{n}}.
$$

(4.94)

where $\alpha_{i\pm1/2,j,k}^{n}$ are again given by Eqs. (4.31)-(4.37). The column vectors $A_{i,j+1/2,k}^{-}$, $B_{i,j\pm1/2,k}^{+}$, and $C_{i,j-1/2,k}^{+}$ are similarly defined. The quantity $D_{N}$ is a $N_{D} \times N_{D}$ diagonal matrix with diagonal elements $(\delta_{11}, \delta_{22}, \ldots, \delta_{N_{D}-1 N_{D}-1}, 0)$. Note that the products $\nu^{e} A^{-}$, $\nu^{e} B^{+}$, $\nu^{e} C^{+}$, and $\omega^{e} D_{N}$ are $7 \times 7$ and $N_{D} \times N_{D}$ influence matrices for the implicit operators of the gas-dynamic and thermodynamic subsystems. Finally, the terms $\nu_{i+1/2,j,k}^{n}$, $\nu_{i,j+1/2,k}^{n}$, $\Delta W_{i+1/2,j,k}^{n}$, $\Delta W_{i,j+1/2,k}^{n}$, $\Delta W_{i,j+1/2,k}^{e}$, $\nu_{i+1/2,j,k}^{n}$, $\omega_{i+1/2,j}^{n}$, $\omega_{i+1/2,j}^{n}$, $\Delta H_{i+1/2,j,k}^{n}$, $\Delta H_{i,j+1/2,k}^{n}$, $N_{w}$, $N_{h}$, $\partial S/\partial Q$, $I$, and $N_{D}$ are as defined for the semi-implicit scheme of Section 4.4.

The unlimited schemes of Chakravarthy and Osher are combinations of second-order central and fully upwind differences. $\theta$ is the parameter that controls the spatial discretization. Values of $\theta = 1/3$, $-1$, $0$, $1/2$, and $1$ result in the third-order, fully-upwind, Fromm's method, low-truncation-error second-order, and central differencing schemes, respectively. A value of $\theta = -1/3$ provides a fifth second-order scheme which does not appear to have a name. The truncation error of the semi-discrete schemes decreases in the order $\theta = -1, 1, -1/3, 0, 1/3, 1/2$. Chakravarthy and Osher [1985a] do not recommend the use of the central-difference or fully-upwind formulations. This is because the unlimited semi-discrete central-difference scheme ($\theta = 1$) is non-dissipative and therefore unreliable, and the fully-upwind scheme ($\theta = -1$) has the greatest truncation error. Chakravarthy and Osher [1985b] also note that Fromm's formulation ($\theta = 0$) provides the highest accuracy in nozzle flow calculations with sonic points.

4.25
4.5.2 Flux Limiters

Like Roe's method, the high-order upwind schemes of Chakravarthy and Osher attain their TVD properties by employing flux limiters. The flux limiters $\phi_i^{\pm n}$ and $\phi_{i+1/2,j,k}^{\pm n}$ are specified by

$$
\phi_{i+1/2,j,k}^{\pm n} = \varphi(b_{i+1/2,j,k}^{\pm n})
$$

where the flux limiter function

$$
\varphi(b) = \max(0, \min(1, \beta b))
$$

is used, $b_{i+1/2,j,k}^{\pm n}$ and $\tilde{b}_{i+1/2,j,k}^{\pm n}$ are flux ratios given by

$$
b_{i+1/2,j,k}^{\pm n} = \frac{\nu_{i-1/2,j,k}^{\pm n}(\Delta W_{i-1/2,j,k}^n \cdot N_{w_k})}{\nu_{i+1/2,j,k}^{\pm n}(\Delta W_{i+1/2,j,k}^n \cdot N_{w_k})},
$$

$$
\tilde{b}_{i+1/2,j,k}^{\pm n} = \frac{\nu_{i+3/2,j,k}^{\pm n}(\Delta W_{i+3/2,j,k}^n \cdot N_{w_k})}{\nu_{i+1/2,j,k}^{\pm n}(\Delta W_{i+1/2,j,k}^n \cdot N_{w_k})},
$$

and $\beta$ is a compression parameter chosen in the interval $0 \leq \beta \leq (3 - \theta)/(1 - \theta)$. If $\beta \geq 1$, higher-order spatial accuracy is obtained. Larger values of $\beta$ result in greater compression of discontinuities. Comparable expressions are used for evaluating the other flux limiters $\phi_{i,j+1/2,k}^{\pm n}$, $\phi_{i,j+1/2,k}^{\pm n}$, $\psi_{i+1/2,j}^{\pm n}$, $\psi_{i+1/2,j}^{\pm n}$, $\psi_{i+1/2,j}^{\pm n}$, and $\tilde{\psi}_{i+1/2,j}^{\pm n}$.

Note that it is possible to use different values of the compression parameter $\beta$ for each characteristic field. Hawken and Gottlieb [1990] found this to be useful for controlling shock resolution and reducing undesirable numerical oscillations. They generally employed smaller values of $\beta$ for the higher-order terms associated with the genuinely nonlinear elemental waves (i.e., for the $k = 1$ and $k = 7$ waves). In some cases, the compression parameter for the nonlinear waves had to be set to values less than unity ($\beta \approx 0.75$) in order to suppress non-physical oscillations.

4.5.3 Entropy or Wavespeed Corrections

The discussion of Section 4.4.4 points out that explicit dissipation, in the form of entropy or wavespeed corrections, must be added to many FDS TVD schemes in order to eliminate nonlinear oscillations and instabilities associated with slowly propagating shocks and blunt-body flow carbuncle phenomena, as well as extraneous or entropy-violating solutions at sonic points. Further attention is also required to ensure that the schemes preserve the positivity of the density (i.e., ensure that the schemes are positively conservative). For high-speed hypersonic flow computations, Yee et al. [1990] have also found that the selection of an entropy correction procedure is particularly important in controlling the stability and steady-state convergence rate of implicit TVD schemes.

**Entropy Correction of Harten**

In the current work, expressions for the wavespeed corrections $\delta\nu$ and $\delta\omega$ are required. One of the more popular entropy correction procedures is due to Harten [1983]. Following
The wave speed correction $\delta \nu_{i+1/2,j,k}^n$ is specified by

$$\delta \nu_{i+1/2,j,k}^n = \frac{\Delta t^n}{J_{i+1/2,j} \Delta \zeta_{i+1/2,j}} \left[ \frac{\left(\lambda_{i+1/2,j,k}^n\right)^2 + \epsilon_k^2}{2 \epsilon_k} - |\lambda_{i+1/2,j,k}^n| \right],$$

(4.99)

where $\epsilon_k$ is a small positive number. Equivalent formulations are used to specify $\delta \omega_{i+1/2,j,k}^n$, $\delta \omega_{i+1/2,j,k}^n$, and $\delta \omega_{i+1/2,j,k}^n$. Suggested values for $\epsilon_k$ are in the range $0 \leq \epsilon_k \leq 0.25$ with a larger value enhancing the entropy enforcement at the expense of solution accuracy (i.e., smearing of discontinuities). This form of wavespeed correction is very effective in preventing the formation of unphysical expansion shocks. It is not, however, effective in reducing the solution wiggles and oscillations for problems with slow-moving shocks and carbuncle phenomena without special tuning of the parameter $\epsilon_k$ [Yee et al., 1990; Lin, 1991]. Furthermore, it is not guaranteed that the resulting modified upwind scheme will be positively conservative [Einfeldt et al., 1991]. Despite these observations, for most unsteady applications as well as stationary subsonic and low-speed supersonic flow problems, the entropy fix suggested by Harten is adequate.

**Wavespeed Correction of Yee, Klopfer, and Montagné**

Yee et al. [1990] have found through a series of numerical experiments that a variable or solution dependent $\epsilon_k$ is required for high-speed stationary flow problems, such as hypersonic blunt-body flows. They suggest $\epsilon_{i+1/2,j,k}$ have the form

$$\epsilon_{i+1/2,j,k} = \bar{\epsilon}_k \left[ |U_{i+1/2,j}^n| + |V_{i+1/2,j}^n| \right]$$

$$+ \frac{a_{i+1/2,j}^n}{2} \left( \sqrt{x_{i+1/2,j}^2 + y_{i+1/2,j}^2} + \sqrt{x_{i+1/2,j}^2 + y_{i+1/2,j}^2} \right),$$

(4.100)

and then the wavespeed correction is given by

$$\delta \nu_{i+1/2,j,k}^n = \frac{\Delta t^n}{J_{i+1/2,j} \Delta \zeta_{i+1/2,j}} \left[ \frac{\left(\lambda_{i+1/2,j,k}^n\right)^2 + \epsilon_{i+1/2,j,k}^n}{2 \epsilon_{i+1/2,j,k}^n} - |\lambda_{i+1/2,j,k}^n| \right],$$

(4.101)

where $\bar{\epsilon}_k$ is a constant ($0.05 < \bar{\epsilon}_k < 0.25$) and $U_{i+1/2,j}^n$, $V_{i+1/2,j}^n$, and $a_{i+1/2,j}^n$ are the appropriate Roe-average values. This wavespeed correction procedure copes with problems involving slow moving shocks and blunt-body flow instabilities and enhances stability and convergence rates for steady-state flow problems; however, it has two drawbacks. Firstly, the explicit dissipation correction of Yee et al. is, in many cases, too diffusive [Lin, 1991]. There is excessive dissipation associated with the linearly degenerate waves which degrades solution quality in regions where it is not required, especially in boundary layers where the pressure gradients are not severe. Secondly, the wavespeed correction does not necessarily result in positively conservative solution methods.

**Wavespeed Correction of Lin**

In an effort to remedy the wavespeed correction procedure of Yee et al. and reduce the dissipation associated with the linear characteristic fields, Lin [1991] has formulated an
alternative expression for \( \epsilon_{i+1/2,j,k}^{n} \) given by

\[
\epsilon_{i+1/2,j,k}^{n} = \left[ |U_{i+1/2,j}^{n}| + a_{i+1/2,j}^{n} \sqrt{x_{i+1/2,j}^{2} + y_{i+1/2,j}^{2}} \right] \left( \tilde{\epsilon}_{k} + \tilde{\kappa}_{k} \kappa_{i+1/2,j,k}^{n} \right),
\]

with

\[
\kappa_{i+1/2,j}^{n} = \frac{1}{4M_{i+1/2,j}^{n}} \left( \frac{|p_{i+1,j}^{n} - 2p_{i+1/2,j}^{n} + p_{i,j-1}^{n}|}{p_{i+1,j}^{n} + 2p_{i+1/2,j}^{n} + p_{i,j}^{n}} + 2 \frac{|p_{i+1,j}^{n} - 2p_{i+1/2,j}^{n} + p_{i+1,j}^{n}|}{p_{i+1,j}^{n} + 2p_{i+1/2,j}^{n} + p_{i+1,j}^{n}} \right),
\]

\[
M_{i+1/2,j,k}^{n} = \begin{cases} 
1, & \sqrt{(u_{i+1/2,j}^{n})^2 + (v_{i+1/2,j}^{n})^2} \leq 1, \\
\frac{\sqrt{(u_{i+1/2,j}^{n})^2 + (v_{i+1/2,j}^{n})^2}}{a_{i+1/2,j}^{n}}, & \sqrt{(u_{i+1/2,j}^{n})^2 + (v_{i+1/2,j}^{n})^2} > 1,
\end{cases}
\]

where \( \tilde{\epsilon}_{k} \) and \( \tilde{\kappa}_{k} \) are positive valued constants. The wave speed correction \( \delta u_{i+1/2,j,k}^{n} \) follows from Eq. (4.101). These equations provide an improved wavespeed correction formulation for the carbuncle phenomenon. The working premise here is that explicit numerical viscosity is necessary for the linear waves to eliminate the instabilities associated with the carbuncle phenomenon (numerical experiments have demonstrated this) but, it is not required in regions where the pressure gradients are small. Note that \( \kappa_{i+1/2,j,k}^{n} \) is proportional to the second difference of the pressure. Lin suggests that \( \tilde{\epsilon}_{1} = \tilde{\epsilon}_{7} = 0.25, \tilde{\epsilon}_{2} = \tilde{\epsilon}_{3} = \tilde{\epsilon}_{4} = \tilde{\epsilon}_{5} = \tilde{\epsilon}_{6} = 0, \tilde{\kappa}_{1} = \tilde{\kappa}_{7} = 5, \) and \( \tilde{\kappa}_{2} = \tilde{\kappa}_{3} = \tilde{\kappa}_{4} = \tilde{\kappa}_{5} = \tilde{\kappa}_{6} = 15, \) although there seems to be some flexibility in the selection of these constants. Lin also notes that the use of non-zero values for \( \tilde{\kappa}_{1} \) and \( \tilde{\kappa}_{7} \) improves convergence.

**Wavespeed Correction of Einfeldt, Munz, Roe, and Sjögreen**

All of the aforementioned entropy or wavespeed correction procedures fail to ensure that the resulting modified Roe-type FDS upwind scheme will be positively conservative [Einfeldt et al., 1991]. Einfeldt et al. have devised a wavespeed modification method that can make the present fully implicit upwind scheme positively conservative. The wavespeed corrections take the form

\[
\delta u_{i+1/2,j,k}^{n} = \frac{\Delta t^{n}}{J_{i+1/2,j} \Delta z_{i+1/2,j}} \left[ \frac{\lambda_{i+1/2,j}^{+n} + \lambda_{i+1/2,j}^{-n}}{2} \right] \left[ \frac{\lambda_{i+1/2,j}^{+n} - \lambda_{i+1/2,j}^{-n}}{2} \right] - 2 (1 - \epsilon_{i+1/2,j,k}^{n}) \frac{\lambda_{i+1/2,j}^{+n} - \lambda_{i+1/2,j}^{-n}}{2} - |\lambda_{i+1/2,j,k}^{n}|,
\]

where

\[
\lambda_{i+1/2,j}^{+n} = \max(\max(\lambda_{i+1/2,j,7}^{n}, \lambda_{i+1/2,j,7}^{n}), 0),
\]

4.28
\[ \lambda_{i+1/2,j}^{-n} = \min(\min(\lambda_{i+1/2,j,1}^{-n}, \lambda_{i,j,1}^{-n}), 0), \quad (4.107) \]

and where
\[ \epsilon_{i+1/2,j,1}^{-n} = \epsilon_{i+1/2,j,7}^{-n} = 0, \quad (4.108) \]

\[ \epsilon_{i+1/2,j,2}^{-n} = \left[ 1 + \frac{\max(\lambda_{i+1/2,j,7}^{-n}, \lambda_{i+1,1,j,7}^{-n}) + \min(\lambda_{i+1/2,j,1}^{-n}, \lambda_{i,j,1}^{-n})}{2 a_{i+1/2,j} \sqrt{n_{i+1/2,j} + y_{i+1/2,j}^2}} \right]^{-1}, \quad (4.109) \]

\[ \epsilon_{i+1/2,j,2} = \epsilon_{i+1/2,j,3} = \epsilon_{i+1/2,j,4} = \epsilon_{i+1/2,j,5} = \epsilon_{i+1/2,j,6}. \quad (4.110) \]

The expressions of Eqs. (4.105)-(4.110) have been derived by considering the numerical flux functions of a Godunov-type scheme developed jointly by Harten, Lax, and van Leer, which is positively conservative. This wavespeed correction procedure provides an effective means by which Roe-type flux Jacobian linearization techniques can be made to handle cases where negative densities and/or internal energies would normally result. The procedure can also serve as a sonic-point entropy fix. Nevertheless, it is important to note that numerical experiments performed as part of the present study indicate that the additional dissipation introduced by the modifications of Einfeldt et al. is not sufficient to damp out oscillations and instabilities in the cases of slow-moving shock and blunt-body flow problems.

**Proposed Wavespeed Corrections**

The preceding observations have lead to a wavespeed correction technique for the proposed factored fully implicit scheme. The wavespeed correction \( \delta \nu_{i+1/2,j,k}^{n} \) is specified herein by
\[ \delta \nu_{i+1/2,j,k}^{n} = \max(\delta \nu_{i+1/2,j,k}^{L,n}, \delta \nu_{i+1/2,j,k}^{E,n}), \quad (4.111) \]

where \( \delta \nu_{i+1/2,j,k}^{L,n} \) is the dissipation correction as suggested by Lin and \( \delta \nu_{i+1/2,j,k}^{E,n} \) is the wavespeed modification devised by Einfeldt et al. described above. Similar expressions are used for evaluating the other wavespeed corrections \( \delta \omega_{i,j+1/2,k}^{n} \), \( \delta \omega_{i+1/2,j,k}^{n} \), and \( \delta \omega_{i,j+1/2,k}^{n} \) and the inclusion of the wave speed corrections in the evaluation of the higher-order antidiffusive fluxes results in a consistent high-resolution scheme. It appears that the modification procedure of Eq. (4.111) offers the desirable dissipation features necessary for preventing unwanted oscillations and instabilities while preserving the positivity of the density. Indeed, several numerical tests (see Figures 4.5-4.8) suggests that this wavespeed correction formulation works well.

**4.5.4 Approximate Factorization Features**

An inspection of Eqs. (4.84), (4.85), (4.87), and (4.88) reveals that, for a given iteration level, the factored implicit solution of the gas-dynamic subsystem only requires the solution of 7 \( \times \) 7 block tridiagonal systems of linear equations in each sweep direction. Moreover, the thermodynamic subsystem does not require the solution of full block tridiagonal systems in either sweep direction. In the \( \eta \)-direction, 2\( N \) scalar tridiagonal systems must be solved for each sweep and, in the \( \zeta \)-direction, the submatrices of the off-diagonal blocks forming the \( N_D \times N_D \) block tridiagonal systems contain only diagonal elements. Although not carried out here, block tridiagonal matrix inversion routines can be devised to account
for the simplified structure of the off-diagonal submatrices and thereby reduce the computational effort required for each \( \zeta \)-sweep. For large thermodynamic systems (i.e., \( N > 5 \)), additional computational savings may be realized if, as suggested by Bussing and Murman [1988], the source Jacobian matrices \( \partial \mathbf{S} / \partial \mathbf{Q} \) are diagonalized by neglecting the off-diagonal influence coefficients. This would simplify the system of linear equations representing each \( \zeta \)-sweep and it would then only be necessary to solve \( N_D \) scalar tridiagonal systems in both sweep directions. All of this make the proposed partially-decoupled fully implicit scheme potentially more attractive than fully coupled factored implicit schemes, which require the solution of \( (2N + 4) \times (2N + 4) \) block tridiagonal systems in both sweep directions.

It has been suggested by Yee and Shinn [1989] that approximate factorization and/or alternating-direction-implicit (ADI) procedures may not be appropriate for the solution of nonequilibrium flows because the stiff source terms can make the factored or ADI algorithm inefficient. However, the observation Yee and Shinn concerned fully coupled solution algorithms. The gas-dynamic subsystem of the present partially-decoupled approach contains only homogeneous terms and the stiff source terms are only present in the thermodynamic subsystem. Furthermore, Molvik and Merkle [1989] have successfully applied a factored implicit scheme to predict nonequilibrium flows and Shih and Chyu [1991] discuss various approximate factorization methodologies for systems of equations with source terms and suggest techniques for reducing the factorization errors when the source terms are large. In the present study, it was found that by choosing the time step so as to maintain the diagonal dominance of the implicit operators of the thermodynamic subsystem and performing subiterations on the thermodynamic subsystem without updating the gas-dynamic subsystem as needed (the capability of performing subiterations on either subsystem for steady or unsteady problems is another computation-saving feature permitted by the partially-decoupled approach), steady-state solutions were obtained within a reasonable number of iterations.

### 4.5.5 Asymptotic Convergence to Steady-State Solutions

Linear stability theory indicates that the solution algorithm of Eqs. (4.83)-(4.89) is unconditionally stable under the following conditions [Beam and Warming, 1982]:

\[
\Omega \geq -\frac{1}{2}, \quad \Theta \geq \Omega + \frac{1}{2}, \quad \Theta \geq \frac{1}{2} \frac{1}{1 + \Omega}.
\]

These inequalities are somewhat misleading because TVD schemes are very often nonlinearly stable even though the underlying unlimited non-TVD version is shown to be linearly unstable [Chakravarthy, 1987]. Moreover, in practice, the time step \( \Delta t^n \) is restricted by linearization and factorization errors. In this study, it was found that optimum CFL numbers \( C_{eff} \) as defined by Eq. (4.57) for steady-state convergence are in the range \( 1 < C_{eff} < 10 \), although even smaller time steps may be required in cases where the source terms are extremely stiff.

Note that it is obviously desirable that the factored fully implicit scheme converge to the time-invariant steady-state solution as rapidly as possible. The numerical experiments of previous studies have established that, although affording excellent solution resolution, Roe flux-difference splitting of the form used herein can give rise to poor convergence rates and limit-cycle behaviour when implemented in implicit time-marching or relaxation schemes for steady-state flow calculations [Mulder and van Leer, 1985; Yee, 1987b; Liou and van Leer, 1988; Yee et al., 1990; Roberts, 1990]. The reasons given for this appear
to be threefold. Firstly, the use of incomplete linearization procedures for evaluating the left-hand-side (LHS) influence matrices of the first-order flux functions arising from the flux-difference splitting procedure (i.e., the assumption used here is that the Roe average state, eigenvalues, and eigenvectors are locally frozen in time) has been shown to lead to limit-cycle behaviour and non-convergence [Mulder and van Leer, 1985; Liou and van Leer, 1988]. Secondly, schemes with higher-order TVD spatial discretization generally have slower steady-state convergence rates [Mulder and van Leer, 1985; Liou and van Leer, 1988; Vee et al., 1990]. This is because the nonlinear manner by which most higher-order TVD schemes minimize dissipation to achieve high-fidelity solutions (i.e., flux limitation) is actually detrimental to convergence. Poor convergence is closely related to the nonlinear flux limiters in these cases [Liou and van Leer, 1988]. Finally, Roberts [1990] argues that the causes of the non-monotone oscillations associated with slow-moving or nearly-stationary shocks may also be a cause for slow rates of convergence of time-marching methods for steady-state applications in which shocks slowly approach their stationary positions.

In most cases, divergence rates of CFD solution schemes may be controlled through the regulation of numerical dissipation. In the present TVD scheme, this can be done through the selection of the compression parameter $\beta$ and other constants associated with the wavespeed correction procedures described in Section 4.5.3. Further control is offered by the choice of time-stepping parameters $\Omega$ and $\Theta$. For viscous hypersonic equilibrium flow computations using implicit time-marching TVD schemes, Yee et al. [1990] indicate that the three-level second-order backward time-stepping procedure ($\Omega = 1/2, \Theta = 1$) is more efficient and stable than the two-level first-order backward Euler method ($\Omega = 0, \Theta = 1$). Note that the use of non-zero $\Omega$ can be viewed as being somewhat analogous to employing an under-relaxation technique. Additional convergence-rate enhancements are possible, such as the local time stepping. The numerical predictions of Chapter 6 will provide a demonstration of the convergence properties of the proposed factored fully implicit TVD algorithm.

### 4.5.6 Local Time Stepping

One simple technique that is used in this study to enhance the steady-state convergence rate performance of the implicit factored method is local time stepping. Spatially-varying time stepping is utilized in which the magnitude of the time step used in the iterative solver at each node of the computational domain is based on the local cell size. This can increase convergence rates, particularly for problems with nonuniform meshes where the ratio of the maximum to the minimum node spacing (cell size) is significantly greater than unity [Pulliam, 1986]. The technique is relatively cheap (i.e., computationally inexpensive) to implement and may aid in improving the convergence properties of the fully implicit solver. In some cases, it was found to be useful in performing the numerical computations of Chapter 6. Note that, in an effort to further enhance convergence rates, a multigrid formulation of the implicit scheme is also considered as part of this work. This multigrid method is described in the next chapter and numerical results are given in Chapter 7.

### 4.6 Boundary Conditions

For both the semi-implicit and fully implicit solvers, boundary conditions are required for prescribing the numerical solution at the extremities of the computational domain. For the example problems considered in the numerical study of this dissertation, two types of approximate boundary conditions are required: a transmissive or nonreflecting outflow...
far-field boundary condition and a reflection or solid-wall boundary condition.

Although sophisticated nonreflecting boundary conditions can be applied by using characteristic extrapolation techniques [Hedstrom, 1979; Thompson, 1987; Kamowitz, 1988], nonreflecting outflow boundary conditions are implemented herein by employing a constant extrapolation technique [Kamowitz, 1988]. If the flux limiters at the boundary node are set to zero, thereby reducing the differencing to first order, this simplified lower-order form of outflow boundary condition is known to permit out-going waves, propagating normal to the boundary, to leave the domain without the formation of unwanted numerical disturbances. The constant extrapolation technique is sufficient for the present calculations; however, for general flows, the approach should be employed with caution. Although the method is appropriate for supersonic outflows in which disturbances cannot travel upstream, the boundary condition is overdetermined and invariably incorrect for subsonic outflow and subsonic and supersonic inflows. This is because the solution state at the boundary is prescribed entirely by the interior solution and does not necessarily correctly represent the physics of the flow outside the numerical grid.

Reflection boundary conditions at solid boundaries are applied by enforcing flow tangency and by employing the frozen-flow Rankine-Hugoniot and Riemann invariant relations across unsteady surface-normal shocks and rarefaction waves to determine the various solution properties. The expressions used depend on the normal flow direction. A description of the analysis for the reflection boundary conditions in the one-dimensional case is given by Gottlieb et al. [1991].

Chakravarthy [1983] has demonstrated that the implicit treatment of boundary conditions improves the convergence rates of finite-difference algorithms used to compute steady-state solutions of the Euler equations. In the proposed factored fully implicit scheme, the constant extrapolation boundary conditions are applied implicitly. However, the reflecting boundary conditions are only applied in an explicit manner.

4.7 Numerical Methods for Thermochemical Equilibrium Flows

As part of the assessment of the proposed numerical schemes for nonequilibrium flow prediction, it was felt that comparisons to numerical results obtained by assuming that the gas is in thermal and chemical equilibrium would be beneficial. Consequently, additional difference schemes were required for the solution of the Euler equations governing inviscid compressible planar flow of equilibrium real gases. The conservation equations of mass, momentum, and energy for this case were introduced in Chapter 3 and are given by Eqs. (3.14)-(3.16). For most equations of state of interest, this system of PDEs is hyperbolic and hence TVD shock-capturing schemes are again appropriate.

Both explicit time-split Roe and factored fully implicit Chakravarthy-Osher upwind methods have been developed for the solution of the equilibrium Euler equations as part of this study. In these FDS methods, the splitting is achieved by employing the approximate Riemann solvers of Appendix A. As the numerical algorithms for the equilibrium case are virtually identical in form to those proposed for the solution of the gas dynamic subsystem of the partially-decoupled nonequilibrium flow equation sets, full details of the solvers are not provided here. Information regarding time splitting, temporal and spatial discretization procedures, linearization and factorization procedures, flux limiting, and entropy corrections can be inferred from the descriptions of the explicit and implicit TVD schemes given in the...
previous sections of the chapter for the gas dynamic subsystem. Note that the solution of the equilibrium flow Euler equations is less complicated than the solution of the decoupled gas dynamic conservation equations because there are fewer PDEs to deal with (four as opposed to seven) and an equation decoupling procedure in not required. Consequently less data storage is needed and the linear systems of equations resulting from the application of the implicit scheme are smaller (4x4 block tridiagonal systems as opposed to 7x7 systems).

4.8 Summary of Numerical Methods

In this chapter, semi-implicit and fully implicit FDS versions of Roe’s and Chakravarthy and Osher’s upwind TVD finite-difference schemes have been described for predicting steady and unsteady, two-dimensional, inviscid flows in thermal and chemical nonequilibrium. The proposed schemes solve the governing hyperbolic conservation laws described in Chapter 3 by means of a partially-decoupled approach. This decoupling procedure is shown to offer many of the computational simplifications and savings of chemistry-split procedures while affording the solution quality of fully coupled algorithms (i.e., the solutions are monotonic as well as preserve the positivity and maximum principles for the mass fractions and discontinuities are handled without excessive smearing). Various features of the methods were outlined including the flux-difference splitting and the rather important wavespeed correction procedures. Similar numerical algorithms were also discussed for gases in thermal and chemical equilibrium where the thermodynamic behaviour can be prescribed by a general equilibrium real-gas EOS. Note that the factored fully implicit solvers of this chapter form the basis of the implicit multigrid TVD methods to be described in Chapter 5.
Figure 4.1: One-dimensional Euler solution to unsteady centered rarefaction wave propagation problem with sonic point at $x=5$ m (air, perfect gas, $\rho_l=1.598$ kg/m$^3$, $u_l=-383.64$ m/s, $p_l=91.88$ kPa, $\rho_r=2.787$ kg/m$^3$, $u_r=-216.97$ m/s, $p_r=200$ kPa). Numerical results for higher-order upwind TVD scheme with Roe flux-difference splitting and without entropy correction illustrating formation of aphysical expansion shock (100 node points).
Figure 4.2: One-dimensional Euler solution to slow leftward propagating shock wave problem with $M_s = 3$ (air, perfect gas, $\rho_l = 1.21 \text{ kg/m}^3$, $u_l = 975.00 \text{ m/s}$, $p_l = 101.10 \text{ kPa}$, $\rho_r = 4.68 \text{ kg/m}^3$, $u_r = 216.36 \text{ m/s}$, $p_r = 1044.70 \text{ kPa}$). Numerical results for higher-order upwind TVD scheme with Roe flux-difference splitting and entropy correction of Harten illustrating persistence of the long-wavelength oscillations behind shock wave (100 node points).
Figure 4.3: One-dimensional Euler solution to unsteady expansion flow problem with leftward and rightward propagating rarefaction waves (air, perfect gas, $\rho_l = 1$ kg/m$^3$, $u_l = -2$ m/s, $p_l = 0.4$ Pa, $\rho_r = 1$ kg/m$^3$, $u_r = 2$ m/s, $p_r = 0.4$ Pa). Numerical results for first-order upwind scheme of Godunov [1959] using an exact Riemann solver (100 node points). TVD upwind schemes using Roe flux-difference splitting fail for this problem without an appropriate choice of wavespeed correction.
Figure 4.4: Two-dimensional Euler solution to steady blunt-body flow about a circular cylinder with $M_\infty = 7.21$ (nitrogen, perfect gas, $p_\infty = 2.08$ kPa, $T_\infty = 1400$ K) showing computed pressure contours. Numerical results for higher-order upwind TVD scheme with Roe flux-difference splitting and entropy correction of Einfeldt et al. illustrating the carbuncle phenomenon ($48 \times 48$ node grid).
Figure 4.5: One-dimensional Euler solution to unsteady centered rarefaction wave propagation problem with sonic point at $x = 5$ m (air, perfect gas, $\rho_l = 1.598$ kg/m$^3$, $u_l = -383.64$ m/s, $p_l = 91.88$ kPa, $\rho_r = 2.787$ kg/m$^3$, $u_r = -216.97$ m/s, $p_r = 200$ kPa). Numerical results for higher-order upwind TVD scheme with Roe flux-difference splitting and wavespeed correction of Eq. (4.111) illustrating removal of aphysical expansion shock (100 node points).
Figure 4.6: One-dimensional Euler solution to slow leftward propagating shock wave problem with $M_s = 3$ (air, perfect gas, $\rho_l = 1.21 \, \text{kg/m}^3$, $u_l = 975.00 \, \text{m/s}$, $p_l = 101.10 \, \text{kPa}$, $\rho_r = 4.68 \, \text{kg/m}^3$, $u_r = 216.36 \, \text{m/s}$, $p_r = 1044.70 \, \text{kPa}$). Numerical results for higher-order upwind TVD scheme with Roe flux-difference splitting and wavespeed correction of Eq. (4.111) demonstrating a reduction of the long-wavelength oscillations behind shock wave (100 node points).
Figure 4.7: One-dimensional Euler solution to unsteady expansion flow problem with leftward and rightward propagating rarefaction waves (air, perfect gas, \( \rho_l = 1 \text{ kg/m}^3 \), \( u_l = -2 \text{ m/s} \), \( p_l = 0.4 \text{ Pa} \), \( \rho_r = 1 \text{ kg/m}^3 \), \( u_r = 2 \text{ m/s} \), \( p_r = 0.4 \text{ Pa} \)). Numerical results for higher-order upwind TVD scheme using Roe flux-difference splitting and wavespeed correction of Eq. (4.111) demonstrating the success of the method for this problem (100 node points).
Blunt-Body Flow over Circular Cylinder, $M=7.21$

48 x 48 Grid

$p$ (kPa)

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Figure 4.8: Two-dimensional Euler solution to steady blunt-body flow about a circular cylinder with $M_\infty = 7.21$ (nitrogen, perfect gas, $p_\infty = 2.08$ kPa, $T_\infty = 1400$ K) showing computed pressure contours. Numerical results for higher-order upwind TVD scheme with Roe flux-difference splitting and wavespeed correction of Eq. (4.111) demonstrating the resolution of the carbuncle phenomenon (48 x 48 node grid).
Chapter 5

Factored Implicit Multigrid TVD
Flux-Difference Split Scheme

5.1 Introductory Remarks

Even though the partially-decoupled factored semi-implicit and fully implicit FDS TVD schemes of Chapter 4 appear to offer reliable, accurate, and relatively efficient means by which to predict high-speed flows predominated by strong shock waves, high temperatures, and thermochemical nonequilibrium processes, such as vibrational relaxation and dissociation and recombination, the computational requirements for solving large systems of nonlinear PDEs with stiff inhomogeneous source terms, such as the one represented by Eqs. (3.8)-(3.10), can still be rather large. Keeping in mind that one of the primary aims of the present study is to develop computationa\textit{ly efficient} schemes, a multigrid solution strategy is proposed in this chapter that employs the partially-decoupled factored implicit TVD scheme of the previous chapter as a smoothing operator. Multigrid or multilevel solution techniques can provide dramatic improvements in steady-state solution convergence rates when compared to single grid computations. The proposed multigrid method may offer a fairly effective means by which to compute steady-state time-invariant solutions of the Euler equations for thermochemical nonequilibrium flow. Some support for this claim is provided by the numerical results of Chapter 7.

The remainder of this chapter is concerned with the development of the factored implicit multigrid TVD FDS scheme for the numerical solution of the conservation laws of Eqs. (3.8)-(3.10) governing two-dimensional inviscid nonequilibrium vibrationally relaxing and chemically reacting flows of thermally-perfect gaseous mixtures. A brief review of multigrid solution techniques is first given followed by details of the proposed method. Descriptions of the multigrid coarse-grid correction procedure, restriction, smoothing, and prolongation operators, as well as various other features of the solution algorithm, are all provided.

5.2 Principles of the Multigrid Method

The multigrid concept has proven to be a powerful and efficient solution technique for boundary-value problems of linear and nonlinear partial differential equations. Although originally developed for elliptic equations [Brandt, 1977], the multigrid method has subsequently been successfully applied to the solution of the hyperbolic PDEs. Multigrid CFD algorithms have been devised for the solution of the Euler equations governing in-
viscid subsonic and transonic compressible flows of perfect gases [Jameson, 1983; Jameson and Mavriplis, 1986; Jameson and Yoon, 1986; Mulder, 1985; Mulder, 1989; Mulder, 1992; Ni, 1982; Yokota and Caughey, 1988]. Furthermore, recent investigations with encouraging results have demonstrated that the technique works for supersonic and hypersonic flows [Decker and Turkel, 1990; Radespiel and Swanson, 1991; Turkel et al., 1991], as well as for chemical nonequilibrium [Bussing and Murman, 1988; Slomski et al., 1990] and viscous flow problems [Cambier and Escande, 1990; Hänel et al., 1989; Yokota, 1990].

In general, multigrid methods can be considered to be enhanced iterative numerical solution methods. It is common to apply iterative techniques in the solution of large matrix systems or for the solution of steady-state boundary value problems of PDEs. The main detraction of many iterative solvers is their sometimes slow convergence rate. Multigrid methods speed up the convergence rates of iterative solvers. This is achieved by reducing the number of mathematical operations required to attain a converged solution. In many cases, total computational effort (times) for multigrid methods are as much as factors of four less than those for the comparable single grid procedure (e.g., [Jameson and Mavriplis, 1986; Jameson and Yoon, 1986; Yokota and Caughey, 1988]).

The fundamental procedure for a multigrid method can be outlined as follows:

(i) **Pre-Smoothing Operator.** Start with an initial estimate of the solution on a fine grid. Apply one or more steps of an iterative solver with appropriate solution error smoothing properties.

(ii) **Restriction Operator.** Transfer the problem, whether it be a linear equation solution problem or a nonlinear partial differential equation solution problem, to a coarser grid.

(iii) **Coarse Grid Solution.** Solve the problem on the coarse grid. As there are fewer grid points in the coarse mesh, the computational costs are reduced.

(iv) **Prolongation Operator.** Transfer the coarse grid solution corrections back to the fine grid in order to generate a better estimate of the fine grid solution. An interpolation procedure is required.

(v) **Post-Smoothing Operator.** Re-apply one or more steps of an iterative solver with appropriate solution error smoothing properties in order to smooth errors possibly introduced by the prolongation process.

(vi) **Multigrid Cycles.** Repeat steps (i) through (v) until convergence. The solution on the coarse grid can be obtained by successively transferring the problem to even coarser grids. Often four and five levels of grids are used and both V- and W-cycles have been proposed. See Figures 5.1 and 5.2.

The procedure outlined above is often called the **coarse-grid correction (CGC)** algorithm due to the fact that corrections to the fine grid solution are obtained from a solution on a coarser grid.

In the basic multigrid method for the iterative solution of a system of linear equations, the multigrid procedure operates on the solution residuals. For nonlinear problems, a full approximate storage (FAS) multigrid is often adopted. The multigrid procedure is then applied to the full iterative solution algorithm (not just the associated linearized equation solution) and operates on the solution itself as well as the residuals. Note that additional
computational advantages may be gained by employing a full multigrid method (FMG) [Radespiel and Swanson, 1991; Turkel et al., 1991] in which the initial guess to the fine grid solution is interpolated from a converged coarse grid solution. In turn, the converged coarse grid solution is obtained from a multigrid procedure with an initial guess interpolated from a converged solution on an even coarser grid. See Figure 5.3 for an illustration of the FMG method. FMG methods are quite analogous to grid or mesh sequencing techniques except that multigrid cycles are performed on each coarse grid.

For elliptic equations, such as Laplace’s equation, the mechanism by which the preceding procedure works can be understood conceptually as follows. In general, iterative solvers for elliptic PDEs are very effective in removing high-frequency (short spatial wavelength) components of the solution error after only a few iterations; however, the solvers take a much greater number of iterations to remove low-frequency (long wavelength) error content. This latter deleterious feature is what slows solution convergence. By transferring the problem to successively coarser meshes, low-frequency errors on the fine grid become high-frequency errors on the coarse grids and are therefore more readily damped. For hyperbolic conservation laws, such as the Euler equations of gas dynamics, the means by which the multigrid method works are slightly different [Gustafsson and Lodstedt, 1989; Decker and Turkel, 1990; Lomax, 1991]. In this case, the physics is dominated by convective wave phenomena and, for low-frequency errors, the multigrid accelerates convergence by permitting the iterative solver (smoothing algorithm) to use large time steps on the coarse grid and thereby allow the rapid transport of transient errors out of the computational domain through nonreflecting boundaries. High-frequency errors, introduced by the solution restriction and prolongation procedure or by the application of boundary conditions, are dissipated on the finer mesh by the iterative solver, as in the elliptic case. It should be evident that, in the elliptic case, smoothing operators with good high-frequency error damping properties are desirable for an effective multigrid method, whereas, in the hyperbolic case, smoothing operators are required that can effectively convect low-frequency errors out of the solution domain and dissipate high-frequency errors created by grid transfers or at the boundaries.

It is hoped that this section has provided a brief overview of some general aspects of multigrid methods. Refer to the references cited for further detailed information.

5.3 Proposed Implicit Multigrid TVD FDS Scheme

In accordance with the preceding ideas and in an effort to improve the convergence to steady-state solutions of the fully implicit TVD algorithm of Chapter 4, a multigrid version of the solution procedure is proposed for the conservation laws of Eqs. (3.8)–(3.10) governing planar two-dimensional high-speed thermal and chemical nonequilibrium flows with strong shocks in terms of a generalized curvilinear coordinate system. The node-centered multigrid algorithm is based on the full FAS and FMG concepts and employs the partially-decoupled factored implicit TVD scheme as the smoothing operator in conjunction with a four-level V-cycle CGC procedure using three coarse grids. A combination simple-injection/full-weighted restriction operator and a bilinear interpolation prolongation operator are used. Algorithmic and procedural details of the proposed multigrid method are given in this section. The basic multigrid procedure used here resembles those developed by Jameson and Yoon [1986] and Caughey [1988]. A similar, although somewhat different, technique has been previously described by Slomski et al. [1990] for chemically reacting flows.
5.3.1 FAS 4-Level V-Cycle FMG Coarse-Grid Correction Procedure

**Smoothing Operator: Partially-Decoupled Factored Implicit TVD Scheme**

Stationary solutions of the Euler equations of Eq. (3.8) are sought via the multigrid method. In the factored fully implicit scheme of Chapter 4, numerical solutions of these conservation equations are obtained by the application of the partially-decoupled approach of Section 4.2 and the subsequent two-stage iterative time-marching solution of the resulting decoupled gas-dynamic and thermodynamic subsystems of Eqs. (4.1) and (4.3) using fully implicit upwind TVD FDS schemes. The two-stage time-marching scheme provides explicit coupling between the gas-dynamic and thermodynamic subsystems. This implicit algorithm is used as the underlying smoothing algorithm in the proposed multigrid method. The high-resolution TVD properties of the schemes should effectively convect low-frequency errors out of the solution domain and the dissipative nature of implicit time stepping should be helpful in removing high-frequency errors created by grid transfers or at the boundaries. Refer to Section 5.3.2 for more on this. Although multi-stage explicit Runge-Kutta time-stepping algorithms have been found to be useful smoothing operators for multigrid methods, particularly when solving inviscid flow problems, Caughey [1988; 1991] suggests that implicit time-stepping schemes may be very effective smoothers for the solution of viscous flows on highly-stretched grids. Moreover, the stiffness of the source terms of the PDEs governing nonequilibrium flows can make explicit time integration procedures very inefficient.

Following the application of the two-level multistep time and TVD FDS upwind spatial discretization procedures and after carrying out the non-conservative first-order linearization procedure, the unfactored form of the fully implicit TVD scheme of Eqs. (4.83)-(4.89) for a given iteration or time level results in two linear systems of equations of the form

\[
Lhs(W_{i,j}^n) \left[ W_{i,j}^{n+1} - W_{i,j}^n \right] = Lhs(W_{i,j}^n) \Delta W_{i,j}^n = Res(W_{i,j}^n),
\]

\[
Lhs(Q_{i,j}^n) \left[ Q_{i,j}^{n+1} - Q_{i,j}^n \right] = Lhs(Q_{i,j}^n) \Delta Q_{i,j}^n = Res(Q_{i,j}^n),
\]

where the superscript \( n \) indicates the iteration level (time step), the subscripts \( i \) and \( j \) are indices for the node points of the discretized computational grid, \( W_{i,j}^n \) and \( Q_{i,j}^n \) are the gas-dynamic and thermodynamic subsystem solution vectors, respectively, \( \Delta W_{i,j}^n \) and \( \Delta Q_{i,j}^n \) are the solution vector changes for the iteration level, \( Lhs(W_{i,j}^n) \) and \( Lhs(Q_{i,j}^n) \) are the left-hand-side (LHS) matrices associated with the linearized implicit operators of the factored implicit TVD schemes, and \( Res(W_{i,j}^n) \) and \( Res(Q_{i,j}^n) \) are the corresponding gas-dynamic and thermodynamic subsystem residuals vectors related to the right-hand-side (RHS) explicit operators of the factored implicit TVD schemes. See Section 4.5 for further details. These two equations will be used to represent the iterative smoothing operator for obtaining the steady-state thermochemical nonequilibrium flow solutions. Note that in the actual iterative scheme, the two systems of equations are not solved directly. Instead, approximate factorization is employed. This reduces the two sets of linear equations to smaller block and scalar tridiagonal systems, which are then solved.

**Coarse Grid Generation**

In the proposed four-level V-cycle FAS multigrid method, four grids are used: one fine grid on which the solution is desired and three coarse grids. As structured gridding and
generalized curvilinear coordinates have been adopted here, the coarse grids are generated by simply eliminating every second line of the fine grid in both curvilinear coordinate directions. This is shown schematically in Figure 5.4. If the multi-level grid sequence is denoted by \( g = 1, \ldots, G \), where \( g = 1 \) is the coarsest grid and \( g = G \) is the finest grid (\( G = 4 \) in the present case), then, using this elimination procedure, the node points of each grid in the physical domain can be related by

\[
x^g_{i/2,j/2} = x^{g+1}_{i,j}, \quad y^g_{i/2,j/2} = y^{g+1}_{i,j},
\]

and the size of each grid is \( I^g \times J^g \) with

\[
I^g = \frac{1}{2} I^{g+1}, \quad J^g = \frac{1}{2} J^{g+1},
\]

where the superscript \( g \) indicates the grid level.

**Restriction Operators**

Restriction operators are required to transfer the iterative problem defined by Eqs. (5.1) and (5.2) to the coarse grids. Like other FAS procedures, the present multigrid method operates on both the solution itself as well as the solution residuals. In general, the restriction operators for the solution and residual vectors may be expressed as

\[
W^g = I_{g+1}^g W^{g+1}, \quad Q^g = I_{g+1}^g Q^{g+1},
\]

\[
\text{Res}(W^g) = I_{g+1}^g \text{Res}(W^{g+1}), \quad \text{Res}(Q^g) = I_{g+1}^g \text{Res}(Q^{g+1}),
\]

where \( I_{g+1}^g \) is the operator for the restriction of the solution from grid levels \( g + 1 \) to \( g \) and \( I_{g+1}^g \) is the corresponding restriction operator for the residuals. As the factored implicit solver is a finite-difference based node-centered scheme, as opposed to a finite-volume based cell-centered method, it is convenient to utilize a simple point-to-point injection procedure to restrict the conserved variables of both the gas dynamic and thermodynamic subsystems. However, a full-weighted restriction procedure is used for the solution residuals of the two subsystems as suggested by Hänöl et al. [1989]. Thus, the restriction operators \( I_{g+1}^g \) for the solution vectors can be expressed very simply as

\[
W^g_{i/2,j/2} = I_{g+1}^g W^{g+1} = W^{g+1}_{i,j}, \quad Q^g_{i/2,j/2} = I_{g+1}^g Q^{g+1} = Q^{g+1}_{i,j}.
\]

The restriction operators \( I_{g+1}^g \) for the residual vectors are more complicated. The restriction operator for the gas-dynamic residuals may be written as

\[
\text{Res}(W^g_{i/2,j/2}) = I_{g+1}^g \text{Res}(W^{g+1}) =
\]

\[
\left[ \frac{J^{g+1}_{i-1,j-1}}{4} \text{Res}(W^{g+1}_{i-1,j-1}) + \frac{J^{g+1}_{i,j-1}}{2} \text{Res}(W^{g+1}_{i,j-1}) + \frac{J^{g+1}_{i+1,j-1}}{4} \text{Res}(W^{g+1}_{i+1,j-1}) + \frac{J^{g+1}_{i-1,j}}{2} \text{Res}(W^{g+1}_{i-1,j}) + J^{g+1}_{i,j} \text{Res}(W^{g+1}_{i,j}) + \frac{J^{g+1}_{i+1,j}}{2} \text{Res}(W^{g+1}_{i+1,j}) \right]
\]

5.5
\[
\begin{align*}
\frac{J_{i,j+1}^{g+1}}{4} \text{Res}(W_{i-1,j+1}^{g+1}) + \frac{J_{i,j}^{g+1}}{2} \text{Res}(W_{i,j+1}^{g+1}) + \frac{J_{i+1,j+1}^{g+1}}{4} \text{Res}(W_{i+1,j+1}^{g+1}) \\
- \left[ \frac{J_{i,j-1}^{g+1}}{4} + \frac{J_{i,j}^{g+1}}{2} + \frac{J_{i+1,j-1}^{g+1}}{4} + \frac{J_{i+1,j}^{g+1}}{2} + J_{i,j}^{g+1} \\
+ \frac{J_{i-1,j}^{g+1}}{4} + \frac{J_{i,j+1}^{g+1}}{2} + \frac{J_{i+1,j+1}^{g+1}}{4} \right],
\end{align*}
\]

(5.8)

where \(J_{i,j}^g\) is the Jacobian of the curvilinear coordinate transformation for grid level \(g\). The restricted residual of Eq. 5.8 is the cell area weighted sum of the residuals performed over the neighboring nine grid points on the finer grid \(g+1\). A similar expression is used for the restriction operator of thermodynamic residuals. In this case, the thermodynamic residuals on the coarse grid are the mass weighted sum of the residuals over the same nine neighboring nodes and given by

\[
\text{Res}(Q_{i/2,j/2}^{g+1}) = \text{Res}(Q_{i,j}^{g+1}) = \\
\left[ \frac{\rho_{i,j-1,j}^{g+1}}{4} \text{Res}(Q_{i-1,j}^{g+1}) + \frac{\rho_{i,j-1,j}^{g+1}}{2} \text{Res}(Q_{i,j-1}^{g+1}) \\
+ \frac{\rho_{i-1,j,j}^{g+1}}{4} \text{Res}(Q_{i-1,j}^{g+1}) + \frac{\rho_{i-1,j}^{g+1}}{2} \text{Res}(Q_{i-1,j}^{g+1}) \\
+ \frac{\rho_{i,j+1,j}^{g+1}}{4} \text{Res}(Q_{i,j+1}^{g+1}) + \frac{\rho_{i,j+1}^{g+1}}{2} \text{Res}(Q_{i,j+1}^{g+1}) \\
+ \frac{\rho_{i+1,j,j}^{g+1}}{4} \text{Res}(Q_{i+1,j}^{g+1}) + \frac{\rho_{i+1,j}^{g+1}}{2} \text{Res}(Q_{i+1,j}^{g+1}) \\
+ \frac{\rho_{i,j}^{g+1}}{2} \text{Res}(Q_{i,j}^{g+1}) \right] / \\
\left[ \frac{\rho_{i,j-1,j}^{g+1}}{4} + \frac{\rho_{i,j-1,j}^{g+1}}{2} + \frac{\rho_{i+1,j,j-1}^{g+1}}{4} + \frac{\rho_{i+1,j}^{g+1}}{2} \right].
\]

(5.9)

It was found that full weighting of the residuals was necessary for good multigrid convergence behaviour.

**Pre- and Post-Smoothing of Solution: Saw-Tooth V-Cycles**

In this FAS multigrid method, the V-cycle CGC scheme depicted in Figure 5.1 is adopted and the multigrid approach is applied to the full iterative solution algorithm. Pre-smoothing of the solution is performed on each successively coarser grid before the restriction process is carried out. However, post-smoothing of the solution is not performed after the prolongation procedure. When post-smoothing of the solution is not carried out, as is the case here, the V-cycles of multigrid methods are sometimes referred to as saw-tooth cycles [Jameson and Yoon, 1986; Catalano and Deconinck, 1990]. Saw-tooth cycles are often employed in multigrid solution techniques for the Euler equations [Ni, 1982; Jameson and Yoon, 1986].

Some numerical experimentation with the present method seems to indicate that the use of two pre-smoothing iterations at each grid level provides good multigrid stability.
and convergence behaviour. Following the suggestions of Radespiel and Swanson [1991],
the higher-order anti-diffusive terms of the Chakravarthy-Osher upwind TVD scheme are
only evaluated on the fine grid and a first-order upwind procedure is employed on each
coarse grid. This is done to enhance the high-frequency spatial error smoothing of the
upwind TVD scheme on the coarse grids, as well as to reduce operation counts per multigrid
cycle. Note also that, although the study of Hänel et al. [1989] shows that convergence of
multigrid methods is directly influenced by the treatment of boundary conditions on the
coarse grids and that the use of frozen boundary conditions is not as effective as the use of
more sophisticated formulations based on FAS concepts, the frozen approximation is utilized
here. Boundary conditions on the coarse grids are not updated. They are only updated on
the fine mesh (i.e., $g = G$). The frozen approach was found to be adequate for the present
work. Nevertheless, improved boundary condition treatment is certainly possible.

Fine-to-Coarse Grid Defect Corrections

In order to maintain the truncation error of the fine grid on each successive coarse grid, fine-
to-coarse grid defect corrections for each subsystem are evaluated as follows. Let $n_g$ be an
index for the pre-smoothing iterations carried out at each grid level $g$ with $n_g = 1, \ldots, N_g$
($N_g = 2$ for the present method). Then, for grid level $g$, the fine-to-coarse grid defect
corrections $\tau_W^g$ and $\tau_Q^g$ are given by

$$
\tau_W^g = \Pi_{g+1}^g Res(W_{g+1}^{g+1, n_g+1} = N_g+1) - \Pi_{g+1}^g Res(W_{g+1}^{g+1, n_g+1} = N_g+1)
= \Pi_{g+1}^g Res(W_{g+1}^{g+1, N_g+1}) - Res(W_{g}^{g, n_g = 1}),
$$

(5.10)

$$
\tau_Q^g = \Pi_{g+1}^g Res(Q_{g+1}^{g+1, n_g+1} = N_g+1) - \Pi_{g+1}^g Res(Q_{g+1}^{g+1, n_g+1} = N_g+1)
= \Pi_{g+1}^g Res(Q_{g+1}^{g+1, N_g+1}) - Res(Q_{g}^{g, n_g = 1}),
$$

(5.11)

where $\Pi_{g-1}^g$ and $\Pi_{g-1}^g$ are again the point-to-point injection and full-weighted restriction
operators for the restriction of the solution and solution residuals, respectively, as defined
above. The superscripts $g$ and $n_g$ indicate the grid and iteration levels, respectively. The
defect corrections of Eqs. (5.10) and (5.11) are often called restriction discretization errors
and can be seen to be the difference between the restricted residuals from the more refined
grid and the residuals evaluated on the current grid. Note that $\tau_W^{G-G} = \tau_Q^{G-G} = 0$. At each
grid level, the defect corrections are used as residual forcing functions in the smoothing
iterations of the nonequilibrium flow solver as follows:

$$
Lhs(W_{i,j}^{g,n_g}) \Delta W_{i,j}^{g,n_g} = Res(W_{i,j}^{g,n_g}) + \tau_{W_{i,j}}^g,
$$

(5.12)

$$
Lhs(Q_{i,j}^{g,n_g}) \Delta Q_{i,j}^{g,n_g} = Res(Q_{i,j}^{g,n_g}) + \tau_{Q_{i,j}}^g.
$$

(5.13)

This all important procedure ensures that the solutions on the coarser grids are driven by
the residuals computed on the fine grid.

5.7
Prolongation Operators

After the smoothing has been performed on the coarsest mesh, gas dynamic and thermodynamic conserved variable solution changes or corrections are prolonged back to successively finer grids using bilinear interpolation in terms of the curvilinear coordinates \( \zeta \) and \( \eta \). This can be defined as follows

\[
W_{g,\text{new}} = W_{g,\text{old}} + I_{g-1}^g \left( W_{g-1,\text{new}} - I_{g-1}^g W_{g,\text{old}} \right),
\]

\[
Q_{g,\text{new}} = Q_{g,\text{old}} + I_{g-1}^g \left( Q_{g-1,\text{new}} - I_{g-1}^g Q_{g,\text{old}} \right),
\]

where \( I_{g-1}^g \) is the interpolation operator and the superscripts \( \text{old} \) and \( \text{new} \) denote the solution before and after the prolongation of the coarse grid corrections.

The interpolation process for the gas-dynamic subsystem solution changes is conducted by bilinearly interpolating the computed corrections for each set of four coarse grid points \((x_{i/2,j/2}^{g-1}, y_{i/2,j/2}^{g-1}), (x_{i/2,j/2+1}^{g-1}, y_{i/2,j/2+1}^{g-1}), (x_{i/2+1,j/2}^{g-1}, y_{i/2+1,j/2}^{g-1}), (x_{i/2+1,j/2+1}^{g-1}, y_{i/2+1,j/2+1}^{g-1})\) on to all fine grid points \((x_{i',j'}, y_{i',j'})\) that are contained within the quadrilateral described by these points. For this node-centered scheme, up to nine fine grid points, including four coincident corner points, can lie within each quadrilateral and \( i' = i, i + 1, \) and \( i + 2, \) and \( j' = j, j + 1, \) and \( j + 2. \) After the technique described by Zingg and Yarrow [1989; 1992], a bilinear mapping of the quadrilateral defined by the four coarse grid points in physical space to the unit square \((0 \leq \zeta_{i',j'} \leq 1, 0 \leq \eta_{i',j'} \leq 1)\) in the transformed or computational plane is assumed having the form

\[
x_{i',j'} = a_x + b_x \zeta_{i',j'} + c_x \eta_{i',j'} + d_x \zeta_{i',j'} \eta_{i',j'},
\]

\[
y_{i',j'} = a_y + b_y \zeta_{i',j'} + c_y \eta_{i',j'} + d_y \zeta_{i',j'} \eta_{i',j'},
\]

where the coefficients of the mapping are given by

\[
a_x = x_{i/2,j/2}^{g-1},
\]

\[
b_x = x_{i/2+1,j/2}^{g-1} - x_{i/2,j/2}^{g-1},
\]

\[
c_x = x_{i/2,j/2+1}^{g-1} - x_{i/2,j/2}^{g-1},
\]

\[
d_x = x_{i/2+1,j/2+1}^{g-1} + x_{i/2,j/2}^{g-1} - x_{i/2+1,j/2}^{g-1} - x_{i/2+1,j/2+1}^{g-1},
\]

\[
a_y = y_{i/2,j/2}^{g-1},
\]

\[
b_y = y_{i/2+1,j/2}^{g-1} - y_{i/2,j/2}^{g-1},
\]

\[
c_y = y_{i/2,j/2+1}^{g-1} - y_{i/2,j/2}^{g-1},
\]

\[
d_y = y_{i/2+1,j/2+1}^{g-1} + y_{i/2,j/2}^{g-1} - y_{i/2+1,j/2}^{g-1} - y_{i/2+1,j/2+1}^{g-1}.
\]

This permits the use of a simple bilinear interpolation formula for the interpolant of the solution changes that can be expressed as

\[
W_{g,\text{new}}^{i',j'} = W_{i',j'}^{g,\text{old}} + a + b \zeta_{i',j'} + c \eta_{i',j'} + d \zeta_{i',j'} \eta_{i',j'},
\]

5.8
where the coefficients of this bilinear function are defined by

\[
a = (W_{g-1, new}^{i,j} - W_{g, old}^{i,j}),
\]

\[
b = (W_{g-1, new}^{i,j} - W_{g, old}^{i,j}) - (W_{g-1, new}^{i,j} - W_{g, old}^{i,j}),
\]

\[
c = (W_{g-1, new}^{i,j+2} - W_{g, old}^{i,j+2}) - (W_{g-1, new}^{i,j} - W_{g, old}^{i,j}),
\]

\[
d = (W_{g-1, new}^{i,j} - W_{g-1, new}^{i+2,j}) + (W_{g-1, new}^{i,j} - W_{g, old}^{i,j})
- (W_{g-1, new}^{i+1,j} - W_{g, old}^{i+1,j+2}) - (W_{g-1, new}^{i+1,j} - W_{g, old}^{i+1,j+2}).
\]  

The values of \(\eta^g_{i,j}\) and \(\eta^g_{i,j}\) necessary for calculating the prolonged solution on the fine grid by means of Eq. (5.26) are determined by solving a quadratic equation that results from Eqs. (5.16) and (5.17) [Zingg and Yarrow, 1989; Zingg and Yarrow, 1992]. A similar prolongation procedure is used for the solution changes of the thermodynamic subsystem except, in this case, density weighted solution corrections are interpolated. The density weighting of the thermodynamic subsystem solution changes is important for maintaining the conservation properties of the numerical solution.

**Summary of Multigrid Method**

The proposed FAS 4-level V-cycle or saw-tooth multigrid method can be summarized using pseudo-code notation as follows:

**Step 1. Pre-smoothing of solution and restriction to coarse grids.**

For \(g = G\) Until \(g = 1\) in Decrements of \(-1\) Do \((G = 4)\)

i) Compute Defect Corrections

If \(g = G\): \(\tau^g_W = 0\)
ELSE: \(\tau^g_W = \Pi_{g+1}^g Res(W_{g+1,N_g+1}^{g,n_g}) - Res(W_{g,n_g=1}^{g,n_g=1})\)
If \(g = G\): \(\tau^g_Q = 0\)
ELSE: \(\tau^g_Q = \Pi_{g+1}^g Res(Q_{g+1,N_g+1}^{g,n_g}) - Res(Q_{g,n_g=1}^{g,n_g}=1)\)

ii) Pre- Smoothing of Solution

For \(n_g = 1\) Until \(n_g = N_g\) in Increments of \(+1\) Do \((N_g = 2)\)

Solve: \(Lhs(W_{i,j}^{g,n_g}) \Delta W_{i,j}^{g,n_g} = Res(W_{i,j}^{g,n_g}) + \tau^g_{W_{i,j}}\)
Solve: \(Lhs(Q_{i,j}^{g,n_g}) \Delta Q_{i,j}^{g,n_g} = Res(Q_{i,j}^{g,n_g}) + \tau^g_{Q_{i,j}}\)

End Do

iii) If \(g \neq 1\) Restrict Solution

\(W_{g-1}^{g-1} = \Pi_{g-1}^{g-1} W^g\), \(Q_{g-1}^{g-1} = \Pi_{g-1}^{g-1} Q^g\)

\(Res(W_{g-1}^{g-1}) = \Pi_{g-1}^{g-1} Res(W^g), Res(Q_{g-1}^{g-1}) = \Pi_{g-1}^{g-1} Res(Q^g)\)

End Do

**Step 2. Prolongation of coarse-grid corrections.**

For \(g = 2\) Until \(g = G\) in Increments of \(+1\) Do \((G = 4)\)

Prolong Solution

\(W_{g,new}^{g} = W_{g,old}^{g} + \Pi_{g-1}^{g} (W_{g-1,new}^{g} - \Pi_{g-1}^{g} W_{g,old}^{g})\)
\(Q_{g,new}^{g} = Q_{g,old}^{g} + \Pi_{g-1}^{g} (Q_{g-1,new}^{g} - \Pi_{g-1}^{g} Q_{g,old}^{g})\)

End Do
Step 3. *Continuation of multigrid solution procedure.* Steps 1 and 2 are repeated until a converged solution on the fine grid \((g = G)\) is attained.

**FMG Strategy**

Further computational advantages are sought by employing a FMG strategy [Radespiel and Swanson, 1991; Turkel et al., 1991] in which the initial guess to the fine grid solution is interpolated from a converged coarse grid solution. In turn, the converged coarse grid solution is obtained from a multigrid procedure with an initial guess interpolated from a converged solution on an even coarser grid. This procedure is illustrated schematically in Figure 5.3. FMG methods are quite analogous to grid or mesh sequencing techniques except that multigrid cycles are performed on each coarse grid.

5.3.2 On the Optimization of Smoothing Properties of the Two-Level Multistep Time-Stepping Procedure

It was noted in the general review of multigrid methods given in Section 5.2 that, for hyperbolic PDEs, effective multigrid smoothing operators should freely convect low-frequency errors out of the solution domain and strongly dissipate high-frequency errors created by grid transfers or at the boundaries. It may be possible to optimize the two-level multistep time-stepping scheme of the present implicit smoother for these purposes by carefully selecting values for the time-stepping control parameters \(\Omega\) and \(\Theta\). As has been done in other studies (e.g., [Jameson and Yoon, 1986; Caughey, 1988; Catalano and Deconinck, 1990; Decker and Turkel, 1990]), the optimization of the smoothing operator may be achieved by turning to Fourier analysis.

For the proposed multigrid method for nonequilibrium flow solution, a possible starting point for the optimization process would be to consider the application of a first-order upwind version of the implicit solution scheme to a simplified one-dimensional model scalar PDE of the form

\[
\frac{\partial u}{\partial t} + \lambda \frac{\partial u}{\partial x} = - Ku ,
\]  (5.31)

where \(\lambda\) and \(K\) are positive valued constants and \(u\) is the dependent variable. Letting \(u^n_i\) be the numerical approximation of the solution to this equation at time \(t = t^n\) and at discrete locations \(x_i\) on a numerical grid with uniform node spacing \(\Delta x = x_{i+1} - x_i\), then the application of the first-order upwind version of the fully implicit solution scheme used in the nonequilibrium flow solver to the model equation results in the following fully-discrete scheme (see Chapter 4):

\[
- \frac{\Theta \nu}{1+\Omega} \Delta u^n_{i-1} + \left[1 + \frac{\Theta (\nu + \kappa)}{1+\Omega} \right] \Delta u^n_i = \frac{\Omega}{1+\Omega} \Delta u^{n-1}_i - \frac{\nu}{1+\Omega} (u^n_i - u^n_{i-1}) - \frac{\kappa}{1+\Omega} u^n_i ,
\]  (5.32)

where \(\Delta u^n_i = u^n_{i+1} - u^n_i\), \(\nu = \lambda \Delta t / \Delta x\), and \(\kappa = K \Delta t\). The now almost classical von Neumann Fourier analysis [Anderson et al., 1984; Hirsch, 1989] can then be performed by assuming that the solution error \(\epsilon\) has the form \(\epsilon^i_j = \exp(c_1 n \Delta t + j c_2 i \Delta x)\), where \(c_1\) and \(c_2\) are Fourier variables and \(j = \sqrt{-1}\), and noting that, as the PDE is linear, the solution error must also satisfy the discrete difference equations. In this way, a quadratic equation
for the amplification factor $\sigma = \exp(c_1 \Delta t)$ can be obtained and written as

$$a\sigma^2 + b\sigma + c = 0,$$

(5.33)

where the coefficients of the quadratic equation are

$$a = 1 + \frac{\Theta \nu}{1 + \Omega} (1 - \cos \phi + j \sin \phi) + \frac{\Theta \kappa}{1 + \Omega},$$

(5.34)

$$b = \frac{(1 - \Theta) \nu}{1 + \Omega} (1 - \cos \phi + j \sin \phi) + \frac{(1 - \Theta) \kappa}{1 + \Omega} - \frac{1}{1 + \Omega},$$

(5.35)

$$c = \frac{\Omega}{1 + \Omega},$$

(5.36)

with $\phi = c_2 \Delta x$. For $\kappa = 0$, stability considerations ensure that $|\sigma| < 1$ for $\Omega \geq 1/2$, $\Theta \geq \Omega + 1/2$, and $\Theta \geq 1/2(1 + \Omega)$ [Beam and Warming, 1982]; nevertheless, within the unconditionally stable regime, it may be possible to optimize $\Omega$ and $\Theta$ such that dispersion (phase) errors are minimized for all wavelengths and so that the damping is large ($|\sigma| \approx 0$) for the highest frequency errors ($\phi \rightarrow \pi$). This, in turn, could result in improved convergence properties for the multigrid method.

Further insight into parameter optimization could be subsequently gained by extending the preceding model equation analysis to two spatial dimensions, as well as by considering higher-order spatial differencing schemes. However, this type of implicit time-stepping parameter optimization procedure has not been performed in the present numerical study. It has been left for future research endeavours. In the present work, implicit Euler time stepping ($\Omega=0$ and $\Theta=1$) is used almost exclusively.

### 5.3.3 Grid-Alignment Problems

For inviscid flow computations, in which coordinate lines of the numerical grid are strongly aligned with the primary flow direction, it has been demonstrated that multigrid techniques are slow to converge (often slower in fact than single-grid techniques) or can even fail to converge due to the occurrence of grid-point decoupling in the direction normal to the flow [Mulder, 1989; Mulder, 1992; Radespiel and Swanson, 1991]. Theoretical reasons for this are offered by Mulder [1988] using two-level Fourier analysis. Grid-alignment problems may be quite significant in the present multigrid method for inviscid thermochemical nonequilibrium flow solution, especially for hypersonic flow problems. Many hypersonic flows are characterized by highly-swept thin shock layers with primary flow directions parallel to slender body surfaces. In the numerical computation of such flows, it is both usual and convenient to choose numerical grids in which the coordinate lines closely follow the hypersonic flow stream lines and, hence, grid-alignment problems can arise. Some numerical experiments are considered in Chapter 7 specifically to illustrate the performance of the proposed multigrid method for problems with flow alignment.

Note that one possible remedy for grid-alignment problems would be the use of a semi-coarsening technique [Mulder, 1989; Mulder, 1992; Radespiel and Swanson, 1991]. Note further that grid alignment is not an issue for viscous flows as it would appear that the presence of viscous terms in the governing flow conservation equations prevent the occurrence of grid-point decoupling.
5.4 Multigrid Method for Thermochemical Equilibrium Flows

A factored implicit multigrid upwind TVD FDS scheme has also been developed for obtaining stationary (time-invariant) solutions to the hyperbolic conservation equations of mass, momentum, and energy that govern inviscid two-dimensional thermal and chemical equilibrium flows of gaseous mixtures with a general real-gas equation of state. This multigrid solution technique for the Euler equations given by Eqs. (3.14)–(3.16) is similar to the multigrid method for nonequilibrium flows described in the preceding sections of this chapter. Therefore, to avoid needless repetition, an algorithm description is not given here.
Figure 5.1: Schematic of multigrid V-Cycles.

Figure 5.2: Schematic of multigrid W-Cycles.
Figure 5.3: Schematic diagram of 4-level full-multigrid V-cycles.
Figure 5.4: Schematic diagram illustrating generation of coarse grid.
Chapter 6

Numerical Results for Semi-Implicit and Fully Implicit Schemes

6.1 Introductory Remarks

The validity of the partially-decoupled semi-implicit and fully implicit TVD FDS algorithms of Chapter 4 is now illustrated by investigating a number of different test flows. The flow problems considered in the assessment include: 1) propagation of one-dimensional planar shocks; 2) quasi-one-dimensional hypersonic impulse tunnel flows; 3) single, complex, and double Mach reflections of planar incident shocks from a wedge in air; 4) the diffraction of a planar high-Mach-number incident shock at an expansion corner in oxygen; 5) supersonic nozzle flow; 6) stationary oblique shock reflection flow of air at a compression ramp; and 7) the steady hypersonic flow of nitrogen over a circular cylinder blunt body. Both nonstationary and stationary flow problems are considered. The unsteady cases of Section 6.4 are useful for validating the semi-implicit solver, and the steady cases of Section 6.5 are used to validate the fully implicit scheme. Many of the flows possess complicated shock structure and most cases exhibit substantial vibrational and chemical nonequilibrium effects. Additionally, many of them have been investigated experimentally, thus making them worthy test problems. Note that some preliminary numerical results have already been presented by Groth and Gottlieb [1991]. Refer to Chapter 7 for numerical results demonstrating the usefulness of the proposed implicit multigrid method of Chapter 5.

6.2 Thermodynamic Models

It was noted in Chapter 3 that the numerical solution of the governing Euler equations requires the prescription of the inhomogeneous source terms representing the finite-rate vibrational relaxation and chemical reaction processes for the gaseous mixture of interest. The test problems considered in this chapter (and the next) involve nonequilibrium flows of air as well as pure oxygen and pure nitrogen. A five-species (N₂, O₂, NO, N, and O) four-temperature (i.e., translational-rotational temperature \( T \), and vibrational energies \( e_{VN_2}, e_{VO_2}, \) and \( e_{VNO} \) ) thermochemical nonequilibrium model for air is used in all of the computations presented here. In this multi-temperature nonequilibrium model, the chemical reaction mechanism of air is represented by seventeen elementary reactions: fifteen dissociation/recombination reactions and two exchange reactions. A Landau-Teller harmonic oscillator formulation is used to model the vibrational relaxation processes. Chemical-vibrational coupling and ionization effects are neglected. The five-species four-temperature
model is valid for temperatures up to 8,000 K and can be used to represent the flows of either pure oxygen or nitrogen by setting the mass concentrations of the other species to zero. The various physical assumptions, mathematical modeling equations, rate constants, and parameters, as well as model limitations, are thoroughly described in Appendix C.

Note that for a number of the flow problems, the nonequilibrium flow results are compared to additional thermochemical equilibrium predictions obtained by assuming that the gaseous mixture, whether it be air, oxygen, or nitrogen, can be described by the well-known polytropic equation of state, \( p = (\gamma - 1)pe \rho RT \) (see Chapter 3). In these cases, the values of \( \gamma \) and \( R \) for air are taken to be 1.40 and 287.06 Pa-m\(^3\)/kg-K, respectively. For oxygen, it is assumed that \( \gamma = 1.40 \) and \( R = 259.82 \) Pa-m\(^3\)/kg-K and, for nitrogen, \( \gamma = 1.40 \) and \( R = 296.80 \) Pa-m\(^3\)/kg-K are used.

### 6.3 Two-Dimensional Grid Generation

In order to solve the two-dimensional test flow problems of this chapter using the proposed solution methods, a procedure is also required for generating the physical coordinates (nodes or mesh points) forming the discretized spatial domains. For the purposes of the present numerical study, a Poisson-equation method is used based on the work of Steger and Sorenson [Steger and Sorenson, 1979; Sorenson, 1980]. This numerical algorithm automates grid point selection and provides a mapping from the physical domain to computational coordinate space. In addition, the grid spacing, orthogonality, and skewness can be controlled by a combination of various algebraic stretching functions that control the distribution of the nodes on the grid boundaries, and by the specification of the source terms of the Poisson-equation mapping that control the relative positions and concentrations of the grid points. The Poisson-equation structured grid generation algorithm is described in considerable detail in Appendix D.

Before continuing, it is felt that a brief discussion of grid resolution requirements and numerical discretization errors is warranted. Thorough and comprehensive grid-refinement studies have not been carried out here to ensure that grid-independent solutions were obtained for all of the stationary and nonstationary two-dimensional problems considered in this chapter. The computations were performed on a Hewlett-Packard/Apollo 400s workstation and the selection of the computational meshes was ultimately dictated by available computational resources. However, it is felt that the numerical solutions are, in most cases, adequately resolved for the purposes of making meaningful comparisons to experiment and for assessing the performance of the solution techniques.

### 6.4 Nonstationary Flow Problems

#### 6.4.1 One-Dimensional Planar Flows

**Shock Wave Propagation in Air**

A first step in the evaluation of the proposed semi-implicit partially-decoupled upwind TVD FDS scheme was to examine the computed numerical solutions for several simple time-dependent one-dimensional problems. In particular, numerical computations of one-dimensional shock waves propagating in air were found to be quite helpful in assessing the effects of stiffness and grid resolution on solution quality. These and other similar one-dimensional calculations also proved to be useful in the selection of the appropriate
computational grids for the two-dimensional problems to follow.

It was noted in Chapter 4 that as the stiffness of a problem increases (i.e., the disparity between the fluid and finite-rate thermochemical time scales increases), more refined spatial meshes and smaller time steps are required in order for a numerical technique to accurately resolve the smallest time and hence spatial scales. In the case of a propagating shock, very refined solution domains are necessary if one is interested in studying the nonequilibrium transition at the shock front. However, for many applications, some form of solution degradation at shocks and reaction fronts is permissible and, as LeVeque and Yee [1990] state, “What we should demand is that the correct discontinuities are obtained. They may be smeared out due to numerical diffusion, but should represent the correct jumps in the correct locations.” Note that it has been shown that some schemes can produce incorrect propagation speeds for discontinuities and that these errors result from a lack of spatial resolution [LeVeque and Yee, 1990; Griffiths et al., 1992].

Consider the one-dimensional problem of a leftward moving $M_s = 8.7$ planar shock wave propagating in air. The pressure, density, and temperature ahead of the shock are 4.097 kPa, 0.0477 kg/m$^3$ and 299.2 K, respectively. The equilibrium flow Mach number behind the incident shock is 2.44 and the equilibrium temperature is approximately 3,320 K. Nonequilibrium effects are prevalent in this flow. The equilibrium post-shock state is about 5–6% dissociated with $c_{N_2} = 0.739$, $c_{O_2} = 0.166$, $c_{NO} = 0.059$, $c_N < 0.001$, and $c_O = 0.035$. This shock propagation problem was solved using the proposed partially-decoupled semi-implicit TVD scheme. Four different solution domains were examined having lengths $L = 5$ cm, 1 m, 20 m, and 400 m, respectively, and, for each of these, four discretized domains were used to obtain the solutions having 25, 50, 100, and 490 uniformly spaced nodal points, respectively. In all cases, the time step was constrained by Eq. (4.57) with a CFL number $CFL = 1/2$. Assuming that the node spacing $\Delta x$ is the characteristic length scale of interest, increasing the length of the solution domain is analogous to increasing the difference between the fluid-dynamic and thermodynamic scales and, hence, the inherent stiffness of the problem. The numerical results for this test case are summarized in Figures 6.1–6.4.

The predictions for $L = 5$ cm are given in Figure 6.1. In this case, the solution domain is such that much of the relaxation process at the shock front can be resolved. The characteristic decay of the temperature, due to a loss in thermal energy through vibrational relaxation and dissociation, and associated rise in the density from their initial values at the shock front to their upstream equilibrium values are evident. The results for $L = 1$ m, 20 m, and 400 m are shown in Figures 6.2, 6.3, and 6.4. As $L$ is increased, the relaxation process following the shock is less resolved until finally, for $L = 400$ m, the front approaches a true discontinuity. Although there is strong evidence of poor solution quality and under-resolution in the 25-node and perhaps 50-node approximate solutions, the 100-node and 490-node solutions are in general agreement and it would appear that the shock is propagated with the correct velocity and solution jumps for all values of $L$. Thus, the partially-decoupled semi-implicit TVD FDS scheme would seem to possess the desirable properties asserted by LeVeque and Yee. A number of other one-dimensional flow calculations have also been performed yielding similar results. Unless the flow was significantly under-resolved, large numerical errors associated with incorrect propagation speeds of discontinuities were not found.

UTIAS-RPI Hypersonic Impulse Tunnel Predictions

In addition to the rather simple one-dimensional exercises of the type just discussed, in a further study, a generalized quasi-one-dimensional nonstationary flow analysis and asso-
ciated TVD finite-difference schemes were developed for predicting the high-temperature flows in the UTIAS-RPI hypersonic impulse tunnel. One-dimensional versions of the proposed semi-implicit nonequilibrium and equilibrium flow solvers were employed and the analysis and computer code were used to investigate the operation and performance of the experimental facility. See Groth et al. [1991]. For completeness, this work is also fully described in Appendix B of the dissertation and detailed numerical results are given therein. The relative success and quality of the tunnel simulation results would seem to demonstrate that the partially-decoupled semi-implicit TVD scheme is fully capable of providing accurate predictions for this class of flows. It should be mentioned that the one-dimensional calculations were very helpful in establishing the nominal operating flow conditions in the nozzle and test section of the UTIAS-RPI facility.

6.4.2 Oblique Shock Reflection Flows

In this section, two-dimensional numerical predictions of the semi-implicit TVD scheme are presented for several different types of nonstationary oblique shock-wave reflections in air and are compared directly to experimental data. In the last ten years, comprehensive experimental and numerical studies of oblique shock-wave reflections in air has been conducted. The experiments were performed by Deschambault and Glass [Deschambault and Glass, 1983; Deschambault, 1984; Glaz et al., 1985; Glaz et al., 1986] using the UTIAS 10-cm by 18-cm hypervelocity shock tube in conjunction with a Mach-Zehnder interferometer. Infinite fringe interferograms of the flowfields were obtained. The corresponding numerical results were computed by Glaz et al. [Glaz et al., 1985; Colella and Glaz, 1985; Glaz et al., 1986; Glaz et al., 1988] using a second-order Eulerian Godunov shock-capturing scheme to solve the conservation laws governing two-dimensional inviscid compressible flow with extensions to include both real-gas equilibrium and high-temperature nonequilibrium effects [Colella and Glaz, 1985; Glaz et al., 1988]. The combined results enhance the understanding of oblique shock reflections and provide an excellent source of benchmark data for the validation of numerical algorithms developed for solving unsteady compressible flow problems with complex nonlinear wave interactions. Note that a number of recent studies (e.g., Needham and Dawson [1989]) have also made direct comparisons between the interferometric results and numerical predictions of other sophisticated shock-capturing schemes.

In most of the shock reflections of the preceding experimental/numerical study, dissociation (and vibrational excitation) effects were negligible and, therefore, the experimental interferograms of Deschambault and Glass provide indirect observations of the two-dimensional flow field density distributions. For non-reacting flows, it can be demonstrated that the fringes of infinite-fringe interferogram interference patterns correspond to actual isopycnics (lines of constant density), and the density difference between any two fringes may be related to the wavelength of the interferometer light source and the Gladstone-Dale constant for the gas. These features make the experimental results particularly useful for code evaluation and were used to advantage by Deschambault and Glass in their comprehensive fringe-counting analysis of the interferogram data. However, for some of the oblique shock reflections considered in the study, the incident shocks were strong and high-temperature effects, including nonequilibrium finite-rate phenomena, were significant [Deschambault, 1984; Glaz et al., 1988].

1For the most part, viscous shear effects are not significant in the unsteady oblique shock reflection flows. Much of the flow field can be assumed to be inviscid. For these reasons, the experimental interferogram data are particularly useful for validating inviscid compressible flow (Euler equation) solvers.

6.4.
Glaz et al., 1986; Glaz et al., 1988]. For these high-Mach-number cases, the thermodynamic behaviour of the air cannot be described by the polytropic equation of state. The presence of dissociation behind the incident and within the reflected shocks means that the fringes of the interferograms no longer correspond to lines of equi-density. Consequently, fringe-counting data reduction techniques become inaccurate and, without the use of an alternative evaluation procedure, interferograms can only provide qualitative information about the flow-field density distribution and shock structure. Some of these limitations were recognized and are indicated by Deschambault [Deschambault, 1984]. Nevertheless, in an effort to provide additional approximate quantitative information concerning the high-temperature flows, the usual fringe-counting analysis was implemented in the previous studies.

For the purposes of the present study, it was felt that the high-Mach-number oblique shock-wave reflection flows considered by Deschambault and Glass, which exhibit substantial nonequilibrium effects, would be very appropriate for assessing the capabilities of the partially-decoupled semi-implicit TVD scheme of Chapter 4. Hence, numerical predictions for four different nonstationary shock reflection flows are investigated herein. However, in order to reduce some of the aforementioned uncertainties associated with comparisons of numerical predictions and experimental results for those cases in which the dissociation of the air was significant and, in turn, to provide a more meaningful qualitative and quantitative evaluation of the semi-implicit method, it was found that re-interpretation of the original experimental data was necessary. This re-interpretation of the interferograms is now discussed and is then followed by the comparisons between numerical and experimental results. Note that the discussion of infinite-fringe interferogram interpretation will more clearly elucidate the problems that arise for chemically reacting flow fields.

Re-Evaluation of Experimental Isopycnics and Computation of Numerical Interferograms

The various components of Mach-Zehnder interferometry system for the UTIAS 10-cm by 18-cm shock tube are depicted in the diagrams of Figure 6.5 [Anderson, 1967; Ben-Dor and Whitten, 1979]. As is typical of such systems, when operating in infinite-fringe mode, the fringe pattern produced by the variation in the light intensity at the viewing screen and at photographic plate of the camera is due to differences in the optical path lengths of the light beams passing through the test section and compensating chamber, respectively. The following formula describes the observed distribution of the light intensity $I$

$$\frac{I}{I_o} = \cos^2 \left[ \frac{\pi \ell(n - n_o)}{\lambda} \right], \quad (6.1)$$

where $I_o$ is a reference value for the intensity, $\lambda$ is the wavelength of the interferometer light source, $\ell$ is the depth of the shock-tube test section, $n$ is the refractive index of the gases in the test section, and $n_o$ is the refractive index of the gases in the compensator. (See Anderson [1967] for further details.) Note that this expression simply represents the time-averaged sum of the intensity of the light beams passing through the test section and compensating chamber. For most non-ionized gaseous mixtures, the refractive index $n$ (and $n_o$) can be related to the density $\rho$ by the Gladstone-Dale relation [Alpher and White, 1959; Anderson, 1967; Ben-Dor and Whitten, 1979]

$$n - 1 = K\rho, \quad (6.2)$$
where $K$ is the specific refractivity or so-called Gladstone-Dale constant.\(^2\) As well, it follows that for a thermally perfect mixture

$$K = \sum s c_s K_s, \quad (6.3)$$

where $c_s$ is the mass concentration of the species $s$ and $K_s$ is the species specific refractivity. In general, the specific refractivity is wavelength dependent (i.e., $K_s = K_s(\lambda)$).

For a non-reacting mixture and monochromatic light, it can be readily deduced from Eqs. (6.1)-(6.3) that each fringe of the interferogram corresponds to an actual isopycnic and the density difference $\Delta \rho$ between any two fringes can be related by

$$\Delta \rho = \frac{\lambda}{K \ell}. \quad (6.4)$$

This expression can be employed in quantitative analyses of the interferograms. However, for the more general case of a mixture that is undergoing chemical reactions such as dissociation and recombination, $K = K(c_s, \lambda)$, the fringe pattern produced by a monochromatic light source corresponds to lines of constant light intensity (iso-intensity lines), and there is no simple expression directly relating the density and fringe spacings (i.e., $\Delta \rho \neq \lambda/K \ell$).

Consider now the experimental data for oblique shock reflections in air. The difficulties associated with the interpretation of the interferograms in the manner adopted by DeSchambault and Glass [Deschambault and Glass, 1983; Deschambault, 1984] are actually three-fold. Aside from the obvious fact that, in the chemically reacting case, the fringes are truly iso-intensity lines and not isopycnics, two other problems or sources of inaccurate interpretation can be identified. Firstly, counting fringes can be problematic as it is not always evident whether a fringe shift is associated with an increase or a decrease in the density. This uncertainty can lead to the incorrect identification of fringes. Secondly, if the fringes are assumed to be isopycnics, then Eq. (6.4) specifies the relative change in the density from one fringe to the next. However, the actual magnitude of some of the fringes must be established in order for the equation to be useful. In the work of Deschambault and Glass, the known incident shock Mach number (a measured quantity) was used in conjunction with three-shock theory for a polytropic gas to predict the values of the flow density at the triple-point of the resulting shock reflection. In the case of strong shocks and high temperatures, the assumption of idealized thermodynamic behaviour becomes invalid and the reference values of the densities obtained from the triple point solution are incorrect. Although there is, in fact, a fringe that corresponds to the frozen jump conditions predicted by the polytropic results, it is virtually impossible to identify.

So the question can be asked, “How can the interferogram data be best used to validate numerical results for cases in which nonequilibrium thermochemical effects are important?”.

One approach to re-interpretating the infinite-fringe Mach-Zehnder interferograms is to re-evaluate the experimental isopycnics. This can be done by first assuming that the state of the air some distance behind the incident shock is equal to the equilibrium state obtained by solving the Rankine-Hugoniot conditions and then by matching one of the experimental fringes within the reflected shock region to an isopycnic from the solution predicted by the

\(^2\)The specific refractivity $K$ is a constant for monochromatic light and nonreacting gaseous mixtures of fixed composition.
Table 6.1: Constants $A_s$ and $B_s$ for Cauchy's dispersion formula.

<table>
<thead>
<tr>
<th>Gas</th>
<th>$A_s$ (m$^3$/kg)</th>
<th>$B_s$ (m$^{-2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>$2.2217 \times 10^{-4}$</td>
<td>$5.67 \times 10^{-15}$</td>
</tr>
<tr>
<td>$N_2$</td>
<td>$2.3251 \times 10^{-4}$</td>
<td>$7.70 \times 10^{-15}$</td>
</tr>
<tr>
<td>$O_2$</td>
<td>$1.8654 \times 10^{-4}$</td>
<td>$5.07 \times 10^{-15}$</td>
</tr>
<tr>
<td>NO</td>
<td>$2.1588 \times 10^{-4}$</td>
<td>$7.40 \times 10^{-15}$</td>
</tr>
<tr>
<td>N</td>
<td>$3.2717 \times 10^{-4}$</td>
<td>$1.474 \times 10^{-15}$</td>
</tr>
<tr>
<td>O</td>
<td>$1.8269 \times 10^{-4}$</td>
<td>$6.336 \times 10^{-15}$</td>
</tr>
</tbody>
</table>

semi-implicit TVD FDS scheme. Although this approach is not fully satisfactory, for it still relies on the assumption that the fringes are isopycnics and uncertainties associated with fringe counting are still present, the technique should provide somewhat improved quantitative information about the experimental flow-field density distribution.

A second approach to re-interpretating the interferograms is to compute a numerical interferogram utilizing Eq. (6.1), i.e., calculate a numerical equivalent of the light intensity field $I/I_0$ at the photographic plate. This is possibly the best approach because it permits direct comparisons to be made between the numerical predictions and experiment. Moreover, it can be argued that agreement between the fringe patterns of the computed and experimental interferograms is a necessary, although not sufficient, condition for establishing agreement between the experimental and predicted flow fields. The concept of computing iso-intensity fields is most certainly not an original idea; however, it seems that the technique is not employed extensively for these types of nonequilibrium flows.

Values of the specific refractive indices $K_s$ are required to calculate a numerical interferogram from the approximate discretized solutions of the flow field density and mass concentrations via Eq. (6.1). In the present work, this means values of $K_s$ for $N_2$, $O_2$, NO, N, and O are needed. Cauchy's dispersion formula [Born and Wolf, 1964; Allen, 1973] is used here. This semi-empirical expression for the specific refractivities has the form

$$K_s = A_s(1 + B_s/\lambda^2),$$

(6.5)

where the constant coefficients $A_s$ and $B_s$ are tabulated for the various species in Table 6.1 [Born and Wolf, 1964; Allen, 1973]. Note that the values of $A_s$ and $B_s$ for monatomic nitrogen, listed in Table 6.1, have been determined herein from measured values for $K_N$ given by Ben-Dor and Whitten [1979]. For interest, the specific refractivities of the various species calculated using Eq. (6.5) are compared in Figure 6.6 to observed values taken from a number of different sources [Hellwege and Hellwege, 1962; Gray, 1972; Alpher and White, 1959; Anderson et al., 1967; Ben-Dor and Whitten, 1979] for a range of wavelengths in the visible spectrum. A $\lambda = 6,943$ Å wavelength light source was used by Deschambault and Glass in all of the experiments that are of concern here.

In summary, two techniques for re-interpretating the interferogram data have been proposed. The experimentally determined isopycnics can be re-evaluated using the procedure suggested above and then compared to the predicted density contours. As well, numerical interferograms or iso-intensity distributions can be computed by means of Eq. (6.1) and then compared directly to the experimental interferograms. In an attempt to provide the
most complete assessment of the flow solver, both of these techniques for re-interpretating the interferogram data are used in the comparisons between the two-dimensional numerical predictions of the semi-implicit TVD scheme and the results of the high-Mach-number oblique shock-wave reflection experiments of Deschambault and Glass which now follow.

**Single Mach Reflection in Air, \( M_s = 2.03 \)**

The first shock reflection problem considered is the oblique reflection of a \( M_s = 2.03 \) planar shock wave propagating in air incident on a 27° compression corner. A schematic diagram of the resulting single Mach reflection pattern is given in Figure 6.7. The incident and reflected shocks, along with the Mach stem and slipstream, are shown. The pressure \( p_0 \) and temperature \( T_0 \) of the quiescent air ahead of the shock are 33.25 kPa and 299.2 K, respectively. The density \( \rho_0 \) is 0.387 kg/m³. The equilibrium flow Mach number and temperature behind the incident shock are about 0.99 and 507 K, respectively. Although nonequilibrium effects are insignificant for this problem, it provides an excellent first test of the capabilities of the gas-dynamic solver for predicting complicated shock structure.

The results pertaining to this test case are shown in Figures 6.8–6.13. The experimental interferogram obtained by Deschambault and Glass is shown in Figure 6.9. In this case, the temperatures are low and each fringe of the interferogram therefore corresponds to an actual isopycnic. The density difference \( \Delta \rho \) between any two fringes can be related by Eq. (6.4) and the corresponding isopycnics, as determined by Deschambault and Glass from an analysis of the interferometric fringe pattern, are given in Figure 6.9.

The single Mach reflection flow problem was solved using the semi-implicit unsteady nonequilibrium flow solution scheme of Chapter 4. A 312×104 node mesh was used in the numerical computation (see Figure 6.8), van Leer’s flux limiter was used for the nonlinear characteristic fields (i.e., \( k = 1 \) and 7 for the gas-dynamic subsystem), and the superbee limiter was employed for the linearly degenerate fields. As is the case for all of the shock reflection and diffraction problems considered herein, the initial data for the computations were specified by locating the incident shock upstream of the corner and by using the Rankine-Hugoniot conditions to prescribe the equilibrium post-shock state. The computed numerical interferogram, obtained with the aid of Eq. (6.1), and the predicted density contours of the single Mach reflection flow field are depicted in Figures 6.10 and 6.11. For reference purposes, this test problem was also solved using the equilibrium flow solver discussed in Chapter 4 with an ideal or polytropic equation of state as discussed above. The results for the polytropic case are given in Figures 6.12. To facilitate comparisons, the values of the labeled density contours of Figures 6.11 and 6.12 are virtually the same as the isopycnics shown Figure 6.9.

By comparing Figures 6.9–6.12, two observations are readily apparent. Firstly, and as anticipated, nonequilibrium high-temperature effects are unimportant here. This is clearly demonstrated by the correspondence between the nonequilibrium predictions of Figure 6.11 and the polytropic calculations of Figure 6.12. Secondly, it would seem that the proposed partially-decoupled semi-implicit TVD scheme is capable of accurately reproducing the general structure of the flow field. The predicted reflected shock is detached from the corner of the wedge, as in the experiment, and its shape is very similar to that of the reflected shock in the interferogram. The position of the triple point appears to be well predicted, as is the slipstream position. Furthermore, the qualitative and quantitative agreement between the two sets of isopycnics is very good. This is true even in the reflected flow region, which can be difficult to predict accurately. These findings are further supported by the additional
comparisons of the predicted and measured distributions of the density along the wall of the compression corner shown in Figure 6.13. The experimental data presented in the wall density distributions have been interpreted from the interferogram. Both original and re-evaluated (see Section 6.4.2) results are given, although there is little difference between the two for this flow. Overall, it can be said that the agreement between calculation and experiment is very good for this first test case.

**Complex Mach Reflection in Air, \( M_s = 10.37 \)**

The next test flow problem considered is the nonstationary oblique reflection of a \( M_s = 10.37 \) planar shock wave propagating in air incident on a 10° compression corner. Again, calculations are compared to the experimental data of Deschambault and Glass. A schematic diagram of the resulting complex Mach reflection pattern is given in Figure 6.14. The incident and reflected shocks along with the Mach stem, slipstream, and kink are all shown. The pressure \( p_o \), density \( \rho_o \), and temperature \( T_o \) ahead of the shock are 6.67 kPa, 0.0777 kg/m³, and 299 K, respectively. Under these conditions, the state of the air behind the incident shock exhibits substantial high temperature effects. The post-shock equilibrium state temperature is about 4,040 K, the flow Mach number is 2.6, and the degree of dissociation of the diatomic molecules is about 10% (\( C_{N_2} = 0.731, C_{O_2} = 0.098, C_{NO} = 0.077, C_N < 0.001, \) and \( C_O = 0.094 \)). One-dimensional calculations, similar to those of Section 6.4.1, indicate that the chemical and vibrational relaxation lengths behind the incident shock are of the order of \( 1-5 \) mm, which is quite large when compared to the dimensions of the experimental flow field [Deschambault, 1984]. Furthermore, Glaz et al. [1988] have demonstrated that a finite-rate nonequilibrium model is required to accurately predict this type of flow.

Results relevant to this complex Mach reflection test case are shown in Figures 6.15–6.20. The experimental interferogram and associated isopycnics for the complex Mach reflection are depicted in Figures 6.16. Note that the values of the isopycnics indicated in the figure are different from those of Deschambault and Glass [1983]. The experimental isopycnics have been re-evaluated using the technique of Section 6.4.2. Although it is recognized that the occurrence of dissociation means the fringes no longer correspond directly to lines of equi-density, as was the case in the previous non-reacting Mach reflection problem, the re-evaluation procedure for the experimental isopycnics still provides some quantitative information about the flow density distribution.

The partially-decoupled semi-implicit scheme was employed in solving this Mach reflection flow field. The 450 \( \times \) 125 node computational mesh of Figure 6.15 and a combination of minmod and superbee limiters were used. The numerical interferogram corresponding to this calculation is depicted in Figure 6.17 and the predicted density contours are displayed in Figure 6.18. As for the single Mach reflection problem, an equilibrium polytropic approximate solution was also computed using an identical numerical grid. This solution is given in Figure 6.19. In contrast to the previous test case, the striking differences between the predicted isopycnics of Figures 6.18 and Figure 6.19 provide strong evidence of thermochemical nonequilibrium phenomena for this flow.

The overall agreement between the nonequilibrium numerical solution and experimental results shown in Figures 6.16–6.18 can be seen to be quite good. The computed and experimental fringes and isopycnics appear to agree both qualitatively and quantitatively. Although there are some numerical disturbances due to startup errors that were also no-
Noticeable in the single Mach reflection solutions, the predicted reflected shock and Mach stem in the nonequilibrium solution are well resolved and the computed slipstream position and associated vortex roll-up compare favourably with experiment. The nonequilibrium simulation predicts that the reflected shock is attached and has a pronounced kink. These features are also observable in the experimental interferogram. Note that the simulation employing the polytropic EOS does not reproduce the kink. Similar agreement can be observed in the wall density plots of Figure 6.20. Notice the disparity between the original interpreted and re-evaluated experimental results in these density profiles.

The exaggerated deformation or toe-out of the base of the Mach stem in the numerical computations of Figures 6.17 and 6.18 is the only major difference between the experimental and simulated flow fields. The deformation is produced by the interaction of the Mach stem and slipstream vortex. Although some curvature of the Mach stem exists in the actual flow, the interaction process is overpredicted in the numerical simulation, and hence the toe-out of the Mach stem is also overpredicted. This discrepancy is attributed to: 1) the absence of viscous effects in the numerical predictions; and 2) the under-resolution of the complicated solution (i.e., insufficient grid refinement) in the Mach stem region. It is conjectured that further refinement of the discretized solution domain and inclusion of viscous effects would improve the predictions. It is informative to note that the quality of the semi-implicit scheme solutions in the Mach stem region was found to be very dependent on four factors: 1) the type of flux limiting used; 2) orthogonality of the grid with respect to the wall; 3) size of the time step; and 4) uniformity of the grid spacing. By employing almost uniform grids that are orthogonal to the wall and by taking the largest time steps permitted by the CFL criterion, numerical diffusion errors are reduced and higher quality solutions are obtained in this region. Some solution tuning is also possible through the choice of flux limiters.

**Double Mach Reflection in Air, \( M_s = 8.7 \)**

The third nonstationary test case considered is also an oblique reflection problem in which a \( M_s = 8.7 \) planar shock wave propagating in air is incident on a 27° compression corner and results in a double Mach reflection pattern. A schematic diagram of this flow field is depicted in Figure 6.21. Primary and secondary reflected shocks, Mach stems, and slipstreams are shown. The pressure, density, and temperature ahead of the shock are 4.097 kPa, 0.0477 kg/m³ and 299.2 K, respectively. Nonequilibrium effects are prevalent in this flow. The equilibrium flow Mach number behind the incident shock is 2.44 and the equilibrium temperature is approximately 3,320 K. The equilibrium post-shock state is about 5–6% dissociated with \( c_{N_2} = 0.739 \), \( c_{O_2} = 0.166 \), \( c_{NO} = 0.059 \), \( c_N < 0.001 \), and \( c_O = 0.035 \). Furthermore, one-dimensional numerical experiments suggest that the nonequilibrium relaxation lengths behind the incident shock are about 3–6 mm. See Section 6.4.1.

Consider Figures 6.22–6.27. The infinite-fringe interferogram of the \( M_s = 8.7 \) double Mach reflection recorded by Deschambault and Glass is illustrated in Figure 6.23. As with the complex Mach reflection, the approximate values of the experimental isopycnics indicated in the figure have been re-evaluated using the procedure described in Section 6.4.2. Shown in Figure 6.24 and Figure 6.25 are the computed interferogram and predicted contours of constant density for this reflection process obtained by employing the partially-

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continuous initial data for the incident shock creates small disturbances which follow behind the shock [Glaz *et al.*, 1985]. Although propagating with the flow velocity and, hence, moving more slowly than the incident shock, these small-amplitude errors are eventually amplified through an interaction with the reflected shock and then pollute somewhat the numerical solution. Remedies for this are possible.
decoupled semi-implicit TVD scheme. The computations were performed using the 486×80 node mesh of Figure 6.22 with the minmod flux limiter applied to all characteristic fields. Similar calculations were also performed assuming ideal-gas behaviour and are displayed in Figure 6.26. Experimental and calculated wall density profiles are given in Figure 6.27.

It can be seen from Figures 6.23–6.27 that high-temperature effects are also important for this flow. Furthermore, the proposed semi-implicit TVD scheme is capable of reproducing both primary and secondary reflected shocks, Mach stems, and slipstreams. The relaxation region directly behind the incident shock also appears to be quite well predicted. Although the toe-out of the Mach stem in the numerical flow field is more evident, in general, the correspondence between numerical and experimental results is again reasonably good.

It is worth mentioning that the characteristic time scales associated with the finite-rate source terms for both the complex and double Mach reflection computations were approximately 100–1,000 times smaller than the gas-dynamic time scales. The semi-implicit solver effectively removed the stability constraints imposed by the finite-rate times scales and permitted the computations to be performed with the numerical time steps controlled only by the gas-dynamic time scales.

Double Mach Reflection in Air, $M_s = 7.19$

One final Mach reflection flow is investigated here. This is the double Mach reflection of a $M_s = 7.19$ planar shock wave propagating in air incident on a 20° compression corner. The resulting reflected shock structure resembles the confluent three-shock double-Mach-stem structure of the preceding case as shown in the schematic diagram of Figure 6.21. The pressure $p_o$ and temperature $T_o$ of the quiescent air ahead of the shock are 8.00 kPa and 298.5 K, respectively. The density $\rho_o$ is 0.093 kg/m$^3$. The equilibrium flow Mach number and temperature behind the incident shock are about 2.18 and 2,675 K, respectively. Numerical and experimental results for this case are given in Figures 6.28–6.32. It can be observed that the results are similar to those shown previously.

6.4.3 Oblique Shock Diffraction Flow

Shock-Wave Diffraction in Oxygen, $M_s = 12$

Another application of the semi-implicit TVD algorithm relates to the prediction of the nonstationary planar flow of dissociated oxygen around a 15° expansion corner. This flow is generated by the diffraction of a $M_s = 12$ planar shock wave. The pressure $p_o$, density $\rho_o$, and temperature $T_o$ of the quiescent oxygen ahead of the shock are 2.67 kPa, 0.0342 kg/m$^3$, and 300 K, respectively. The frozen flow Mach number behind the shock is 2.7 and the temperature is about 3,825 K. The post-shock state of the oxygen is approximately 23% dissociated. The classical shock-wave diffraction pattern is shown in the diagram of Figure 6.33. The figure illustrates the Prandtl-Meyer expansion wave and the recompression shock and associated contact surface. A strong nonequilibrium recombination process occurs through the rarefaction wave fan after the high-Mach-number shock passes the corner.

The shock diffraction problem was computed using the semi-implicit TVD algorithm and a 308×156 node grid (see Figures 6.34). A combination of the van Leer and superbee flux limiters was used. The predicted density contours at a time 26.5 $\mu$s after the shock has passed the corner are given in Figures 6.35. The recompression shock and contact surface are clearly evident in the figure and appear to be well resolved. The fan of the stationary rarefaction wave evolving from the corner can also be observed.
An experimental study of the flow of dissociated oxygen around expansion corners was carried out by Drewry [Drewry, 1967; Glass, 1967] in the UTIAS 10-cm by 18-cm hypervelocity shock tube. Comparisons of the predicted isopycnics of Figures 6.35 to schlieren photographs (Fig. 33a and Fig. 35 of Drewry [1967]) reveal that the general features of the flow field are duplicated by the present numerical method, including the shapes and relative positions of the recompression shock and contact surface. The predicted angles of the head and tail of the rarefaction wave relative to the horizontal also agree with the respective values of 20° and 1°-2° reported by Drewry.

Experimental measurements of the wall density distribution were also made by Drewry using finite-fringe Mach-Zehnder interferometry. (The actual density values were interpreted from the fringe shifts.) However, these data are not included in the comparisons due to uncertainties in the interpretation of the experimental results. Unfortunately, the measured densities were clearly influenced by the presence of a wall boundary layer and viscous effects.

6.5 Stationary Flow Problems

6.5.1 Supersonic Nozzle Flow of Air

Three stationary flow problems are now considered in order to provide some assessment of the factored fully implicit partially-decoupled upwind TVD FDS scheme. The first problem is the steady supersonic flow of air through a planar two-dimensional diverging nozzle, 2 m in length, with an exit to entrance area ratio of 9.1 (see Figure 6.36). The axial flow at the nozzle entrance is taken to be supersonic, uniform, and in thermal and chemical equilibrium. The entrance conditions are: $M_e = 1.5; p_e = 101.325\, \text{kPa};$ and $T_e = 6,000\, \text{K}$. The flow is smooth and shockless. However, nonequilibrium finite-rate processes occur as the air expands through the diverging nozzle.

This supersonic nozzle flow problem was solved using the fully implicit algorithm. For comparative purposes, both thermochemical nonequilibrium and ideal-gas solutions were determined. A $64 \times 32$ computational grid was employed; see Figure 6.37. The values of the time stepping, spatial differencing, and compression control parameters used in the calculations were $\Theta = 1, \Omega = 0, \theta = 0,$ and $\beta = 1$, respectively. A CFL number of five was utilized ($C_{cfl} = 5$). Uniform initial data were assumed in order to initiate the time-marching solution procedures and the convergence of the solution was inferred by monitoring the residual $\epsilon = \sum_i |\Delta p_i|/(N_p\rho_i)$, where $N_p$ is the total number of nodes in the discretized domain. It was assumed that an approximate steady-state solution was obtained when the residual was reduced by five orders of magnitude from its initial value. This occurred within 220-250 iterations or time steps. The convergence history of the nonequilibrium flow solution is presented in Figure 6.41.

The numerical results pertaining to this test case are shown in Figures 6.38-6.40. The computed nonequilibrium flow solution for the distribution of the translational-rotational temperature $T$ in the nozzle is indicate in the contour plot of Figure 6.38. The corresponding equilibrium temperature distribution for the ideal case is depicted in Figure 6.39. The characteristic decrease in the flow temperature along the centre-line or axis of the nozzle is clearly illustrated in Figure 6.40. Note the differences between the polytropic and nonequilibrium solutions. Although experimental data for comparison are not available, the computed solutions are typical of supersonic nozzle flows and it would seem that the partially-decoupled fully implicit method is capable of providing adequate results for this class of nonequilibrium flows.
6.5.2 Compression Ramp Flow in Air, \( M_\infty = 22 \)

The next stationary problem studied is the oblique shock reflection flow of air at a compression ramp with a free-stream Mach number of \( M_\infty = 22 \) and a wedge angle of 20°. Refer to Figure 6.42. Standard atmospheric conditions at an altitude of 42 km are used for the free-stream conditions. The pressure \( p_\infty \), temperature \( T_\infty \), and density \( \rho_\infty \) corresponding to this altitude are 0.21997 kPa, 255.88 K, and 0.00299 kg/m³, respectively. Such conditions would be typical for hypersonic flight. It is also assumed that the free stream is composed entirely of diatomic nitrogen and oxygen with \( c_{N_2} = 0.767 \) and \( c_{O_2} = 0.233 \). This problem was investigated in a previous study by Slomski et al. [1990] using a thermal equilibrium chemical nonequilibrium model.

A solution to this problem was computed using the factored fully implicit partially-decoupled TVD scheme on the 96 x 40 grid. The computational mesh is illustrated in Figure 6.43. The time stepping control parameters used were \( \Theta = 1 \) and \( \Omega = 0 \), the spatial differencing control parameter was \( \theta = 0 \) (Fromm’s method), and a value of \( \beta = 1 \) was used for the compression parameter for the flux limiters. Time step selection corresponded to a CFL number of \( C_{eff} = 2 \). A uniform free stream was assumed for the initial data. Roughly 300-350 iterations were required to reduce the solution residual measure, \( \epsilon = \sum |\Delta \rho_i|/(N_p \rho_i) \), by five orders of magnitude and to achieve the required steady-state result.

The contours of the translational-rotational temperature \( T \) for the converged solution, showing a predicted shock angle of about 23°, are depicted in Figure 6.44. For interest sake, a similar numerical result is shown in Figure 6.45 for the case of a polytropic gas. The wall temperature profiles for both computations are presented in Figure 6.46. Solution convergence is indicated in the plots of Figure 6.47 as a function of the number of implicit time steps or iterations.

It is evident from Figures 6.44–6.46 that nonequilibrium effects are significant in the computed flow field behind the oblique shock. An ideal gas is less compressive and, hence, the angle of the oblique shock in the polytropic solution is greater than the angle that can be observed in the nonequilibrium solution. There is also a very long protracted thermochemical nonequilibrium relaxation process occurring downstream of the shock in the finite-rate solution. The physical length of the computational domain in the primary flow direction is 20 m. The predicted post-shock state, very close to the ramp wall, has a translational-rotational temperature that varies from about 4,300–4,400 K just past the corner to about 3,050 K at the edge of the domain downstream of the corner. Stationary oblique shock theory predicts that the post-shock temperature and shock angle should be about 4,423 K and 24.6°, respectively, if the air is assumed to be thermally and chemically frozen, and approximately 2,900 K and 23°, if thermodynamic equilibrium is assumed. At the equilibrium temperature, the air is about 4% dissociated with \( c_{N_2} = 0.75 \), \( c_{O_2} = 0.17 \), \( c_{N_0} = 0.04 \), \( c_N < 0.001 \), and \( c_O = 0.04 \). It would appear that the factored implicit algorithm performs well for this test case. The shock is well resolved as is the relaxation process occurring downstream of the shock. Furthermore, the solution converges fairly rapidly.

6.5.3 Blunt-Body Flow in Nitrogen, \( M_\infty = 6.9 \)

The final test case considered in the evaluation of the proposed TVD schemes is a hypersonic blunt-body flow around a two-dimensional circular cylinder with its axis of symmetry perpendicular to the free-stream flow direction such that a stationary bow shock forms about the body (see the schematic of Figure 6.48). The free-stream gas is pure nitrogen and the
radius of the cylinder is 2.54 cm. The thermodynamic state of the free-stream nitrogen is such that the gas is 7% dissociated (i.e., $c_{N_2} = 0.93$ and $c_N = 0.07$). The free-stream pressure $p_\infty$, density $\rho_\infty$, temperature $T_\infty$, and velocity $u_\infty$ are 2.445 kPa, $5.50 \times 10^{-3}$ kg/m$^3$, 1400 K, and 5.5 km/s, respectively. The frozen-flow free-stream Mach number is about 6.9.

This blunt-body flow was investigated experimentally by Hornung [1972; 1976]. The infinite-fringe interferogram of the flow field recorded by Hornung using Mach-Zehnder interferometry is given in Figure 6.50. A strong nonequilibrium dissociation process occurs following the bow shock and thermal equilibrium conditions are reached in the vicinity of the stagnation point where flow Mach numbers are small. Recent numerical studies have shown that a nonequilibrium analysis is required to accurately predict the density distribution and shock standoff distance for this flow [Park and Yoon, 1991]. The problem is therefore quite appropriate for assessing the fully implicit TVD algorithm.

The preceding blunt-body flow problem was solved by using the fully implicit partially-decoupled TVD scheme on a 96x96 grid. The mesh used is given in Figure 6.49. The time-stepping, spatial differencing, and compression control parameters used for the calculation are as follows: $\Theta = 1$; $\Omega = 0$; $\theta = 0$; and $\beta = 0.75$. A uniform free stream was assumed for the initial data and the computations were carried out until the measure of the solution residual, $\epsilon = \sum_i |\Delta \rho_i|/(N_p \rho_i)$, was reduced by three orders of magnitude and velocity of the bow shock approached zero. About 2,500 iterations were required to achieve the approximate steady-state solution with the size of the time steps corresponding to a CFL number of two ($C_{fl} = 2$). Shown in Figure 6.51 are the isopycnics of the numerical solution. The variation of the translational-rotational temperature $T$ along the stagnation streamline is illustrated in Figure 6.52. Solution convergence is depicted in Figure 6.53.

A number of observations can be made concerning the numerical results for this test case. The nonequilibrium thermochemical relaxation process following the bow shock is clearly indicated in Figure 6.52. The predicted stagnation temperature and density are approximately 6,600 K and 0.066 kg/m$^3$, respectively, and the nitrogen is found to be 23% dissociated near stagnation ($c_{N_2} = 0.77$ and $c_N = 0.23$). Although the fringes of the experimental interferogram do not represent the actual isopycnics, a comparison of Figures 6.49 and 6.51 reveals that the numerical results closely resemble the experimental flow field. The bow-shock standoff distance and shape are both well predicted. Some of the finer details of the density distribution also seem to be reproduced by the fully implicit TVD scheme.

### 6.6 Summary of Numerical Results

The numerical results presented in this chapter (and in Appendix B) provide substantial validation of the proposed partially-decoupled flux-difference splitting approach, as well as a verification of the associated upwind TVD algorithms. From the nonstationary flow calculations, it is readily apparent that the semi-implicit method is very capable of predicting complex unsteady nonequilibrium flows with complicated shock structure. It was also found that re-interpretation of oblique shock reflection interferogram data was essential for the effective comparison of predicted nonequilibrium flow fields and experimental results. Although solution convergence for the blunt-body flow problem was somewhat slower than the other two stationary cases, it would also appear that the factored fully implicit algorithm can provide higher-order accurate approximate steady-state solutions within a reasonable number of iterations.
Figure 6.1: One-dimensional unsteady leftward propagating shock wave problem; $M_s = 8.7$, $p_0 = 4.097$ kPa, $T_0 = 299.2$ K, $L = 5$ cm. Numerical results illustrating effects of grid resolution (25, 50, 100, 490 node points).
Figure 6.2: One-dimensional unsteady leftward propagating shock wave problem; \( M_s = 8.7, p_o = 4.097 \text{ kPa}, T_o = 299.2 \text{ K}, L = 1 \text{ m}. \) Numerical results illustrating effects of grid resolution (25, 50, 100, 490 node points).
Figure 6.3: One-dimensional unsteady leftward propagating shock wave problem; $M_s = 8.7$, $p_o = 4.097 \text{kPa}$, $T_o = 299.2 \text{K}$, $L = 20 \text{m}$. Numerical results illustrating effects of grid resolution (25, 50, 100, 490 node points).
Figure 6.4: One-dimensional unsteady leftward propagating shock wave problem; $M_s = 8.7$, $p_0 = 4.097$ kPa, $T_0 = 299.2$ K, $L = 400$ m. Numerical results illustrating effects of grid resolution (25, 50, 100, 490 node points).
Figure 6.5: Schematic diagrams of UTIAS Mach-Zehnder Interferometer.
Figure 6.6: Specific refractivity $K$ of various gases as a function of wavelength $\lambda$. 
Figure 6.7: Schematic diagram of single Mach reflection; I, incident shock; R, reflected shock; M, Mach stem; S, slipstream.

Figure 6.8: 312 x 104 computational grid used in single Mach reflection prediction; $M_s = 2.03$, $\theta = 27^\circ$, $p_o = 33.25$ kPa, $T_o = 299.2$ K. Every fourth grid line is shown.
Figure 6.9: Single Mach reflection; $M_s = 2.03$, $\theta = 27^\circ$,
$p_o = 33.25$ kPa, $T_o = 299.2$ K. Interferogram
and experimentally determined isopyncnics.

$\rho/\rho_o$ 1 1.00 5 2.73 9 3.49 D 3.80 H 4.12
2 1.50 6 3.00 A 3.57 E 3.88 I 4.20
3 2.00 7 3.40 B 3.65 F 3.96
4 2.50 8 3.41 C 3.73 G 4.04

Figure 6.10: Single Mach reflection; $M_s = 2.03$, $\theta = 27^\circ$,
$p_o = 33.25$ kPa, $T_o = 299.2$ K. Computed
numerical interferogram.
Figure 6.11: Single Mach reflection; $M_s = 2.03, \theta = 27^\circ$, $p_o = 33.25\, \text{kPa}$, $T_o = 299.2\, \text{K}$. Predicted constant density contours.

Figure 6.12: Single Mach reflection; $M_s = 2.03, \theta = 27^\circ$, $p_o = 33.25\, \text{kPa}$, $T_o = 299.2\, \text{K}$. Predicted constant density contours, polytropic gas.
Figure 6.13: Single Mach Reflection; $M_s = 2.03$, $\theta = 27^\circ$, $p_o = 33.25$ kPa, $T_o = 299.2$ K. Predicted and measured wall density distributions.
Figure 6.14: Schematic diagram of complex Mach reflection:
I, incident shock; R, reflected shock;
M, Mach stem; S, slipstream; K, kink.

Figure 6.15: 450 × 125 computational grid used in complex
Mach reflection prediction; $M_s = 10.37$,
$\theta = 10^\circ$, $p_o = 6.67$ kPa, $T_o = 299$ K.
Every fourth grid line is shown.
\[
\begin{array}{ccccccccccc}
\rho/\rho_o & 1 & 1.00 & 5 & 8.73 & 9 & 10.64 & D & 12.19 & H & 13.74 \\
2 & 2.00 & 6 & 8.72 & A & 11.03 & E & 12.58 & I & 14.12 \\
3 & 4.00 & 7 & 9.11 & B & 11.42 & F & 12.96 & J & 14.51 \\
4 & 6.00 & 8 & 9.67 & C & 11.80 & G & 13.35 \\
\end{array}
\]

Figure 6.16: Complex Mach Reflection; \( M_s = 10.37, \theta = 10^\circ, \)
\( p_o = 6.67 \text{ kPa}, T_o = 299 \text{ K}. \) Interferogram and experimentally determined isopycnics.

\[
\begin{array}{ccccccccccc}
\rho/\rho_o & 6.00 & 8 & 9.67 & C & 11.80 & G & 13.35 \\
\end{array}
\]

Figure 6.17: Complex Mach Reflection; \( M_s = 10.37, \theta = 10^\circ, \)
\( p_o = 6.67 \text{ kPa}, T_o = 299 \text{ K}. \) Computed numerical interferogram.
Figure 6.18: Complex Mach Reflection; \( M_s = 10.37, \theta = 10^\circ \),
\( p_0 = 6.67 \text{ kPa}, T_0 = 299 \text{ K} \). Predicted
constant density contours.

Figure 6.19: Complex Mach Reflection; \( M_s = 10.37, \theta = 10^\circ \),
\( p_0 = 6.67 \text{ kPa}, T_0 = 299 \text{ K} \). Predicted
constant density contours, polytropic gas.
Figure 6.20: Complex Mach Reflection; $M_s = 10.37$, $\theta = 10^\circ$, $p_0 = 6.67$ kPa, $T_0 = 299$ K. Predicted and measured wall density distributions.
Figure 6.21: Schematic diagram of double Mach reflection; I, incident shock; R, R', reflected shocks; M, M' Mach stems; S, S' slipstreams.

Figure 6.22: $486 \times 80$ computational grid used in double Mach reflection prediction; $M_s = 8.7$, $\theta = 27^\circ$, $p_o = 4.097$ kPa, $T_o = 299.2$ K. Every fourth grid line is shown.
Figure 6.23: Double Mach Reflection; $M_s = 8.7$, $\theta = 27^\circ$, $p_o = 4.097$ kPa, $T_o = 299.2$ K. Interferogram and experimentally determined isopycnics.

Figure 6.24: Double Mach Reflection; $M_s = 8.7$, $\theta = 27^\circ$, $p_o = 4.097$ kPa, $T_o = 299.2$ K. Computed numerical interferogram.
Figure 6.25: Double Mach Reflection; $M_s = 8.7$, $\theta = 27^\circ$, $p_0 = 4.097$ kPa, $T_o = 299.2$ K. Predicted constant density contours.

Figure 6.26: Double Mach Reflection; $M_s = 8.7$, $\theta = 27^\circ$, $p_0 = 4.097$ kPa, $T_o = 299.2$ K. Predicted constant density contours, polytropic gas.
Figure 6.27: Double Mach Reflection; $M_s = 8.7$, $\theta = 27^\circ$, $p_o = 4.097$ kPa, $T_o = 299.2$ K. Predicted and measured wall density distributions.
Figure 6.28: 486 × 80 computational grid used in double Mach reflection prediction; $M_s = 7.19$, $	heta = 20^\circ$, $p_o = 8.00$ kPa, $T_o = 298.5$ K. Every fourth grid line is shown.
Figure 6.30: Double Mach Reflection; $M_s = 7.19$, $\theta = 20^\circ$, $p_o = 8.00$ kPa, $T_o = 298.5$ K. Predicted numerical interferogram.
Figure 6.31: Double Mach Reflection; $M_s = 7.19, \theta = 20^\circ$, $p_o = 8.00 \text{ kPa}, T_o = 298.5 \text{ K}$. Predicted constant density contours.
Figure 6.32: Double Mach Reflection; $M_a = 7.19$, $\theta = 20^\circ$, $p_o = 8.00$ kPa, $T_o = 298.5$ K. Predicted and measured wall density distributions.
Figure 6.33: Schematic diagram of shock-wave diffraction at an expansion corner; I, incident shock; R, rarefaction fan; S, recompression shock; C, contact surface.

Figure 6.34: $308 \times 156$ computational grid used in shock-wave diffraction prediction; $M_s = 12$, $\theta = 15^\circ$, $p_o = 2.67$ kPa, $T_o = 300$ K. Every fourth grid line is shown.
Figure 6.35: Shock-wave diffraction; $M_s = 12$, $\theta = 15^\circ$, $p_o = 2.67$ kPa, $T_o = 300$ K. Predicted constant density contours.
Figure 6.36: Schematic diagram of supersonic diverging nozzle flow.

Figure 6.37: 64 x 32 computational grid used in supersonic diverging nozzle flow prediction; $M_e = 1.5$, $y/y_e = 9.1$, $p_e = 101.325$ kPa, $T_e = 6,000$ K.
Figure 6.38: Supersonic diverging nozzle flow; $M_e = 1.5$, $y/y_e = 9.1$, $p_e = 101.325$ kPa, $T_e = 6,000$ K. Predicted constant temperature contours.

Figure 6.39: Supersonic diverging nozzle flow; $M_e = 1.5$, $y/y_e = 9.1$, $p_e = 101.325$ kPa, $T_e = 6,000$ K. Predicted constant temperature contours, polytropic gas.
Figure 6.40: Supersonic diverging nozzle flow; $M_e = 1.5$, $y/y_e = 9.1$, $p_e = 101.325$ kPa, $T_e = 6,000$ K. Predicted centre-line temperature profile.

Figure 6.41: Supersonic diverging nozzle flow; $M_e = 1.5$, $y/y_e = 9.1$, $p_e = 101.325$ kPa, $T_e = 6,000$ K. Solution convergence.
Figure 6.42: Schematic diagram of compression ramp flow; S, reflected shock.

Figure 6.43: 96 x 40 computational grid used in hypersonic compression ramp flow prediction; \( M_\infty = 22, \theta = 20^\circ, p_\infty = 0.21997 \text{ kPa}, T_\infty = 255.88 \text{ K}. \)
Figure 6.44: Compression ramp flow; $M_\infty = 22$, $\theta = 20^\circ$, $p_\infty = 0.21997$ kPa, $T_\infty = 255.88$ K. Predicted constant temperature contours.

Figure 6.45: Compression ramp flow; $M_\infty = 22$, $\theta = 20^\circ$, $p_\infty = 0.21997$ kPa, $T_\infty = 255.88$ K. Predicted constant temperature contours, polytropic gas.
Figure 6.46: Compression ramp flow; \( M_\infty = 22, \theta = 20^\circ, \)
\( p_\infty = 0.21997 \text{ kPa}, T_\infty = 255.88 \text{ K}. \) Predicted
wall temperature profile.

Figure 6.47: Compression ramp flow; \( M_\infty = 22, \theta = 20^\circ, \)
\( p_\infty = 0.21997 \text{ kPa}, T_\infty = 255.88 \text{ K}. \) Solution
convergence.
Figure 6.48: Schematic diagram of blunt-body flow over circular cylinder; C, circular cylinder; S, bow shock.

Figure 6.49: 96 × 96 computational grid used in hypersonic blunt-body flow prediction; $u_\infty = 5.5$ km/s, $r = 2.54$ cm, $\rho_\infty = 5.5 \times 10^{-3}$ kg/m$^3$, $T_\infty = 1,400$ K. Every second grid line is shown.
Figure 6.50: Blunt-body flow; \( u_\infty = 5.5 \text{ km/s} \), \( r = 2.54 \text{ cm} \), \( \rho_\infty = 5.5 \times 10^{-3} \text{ kg/m}^3 \), \( T_\infty = 1,400 \text{ K} \).

Interferogram taken from Hornung [1976], Fig. 4.
Figure 6.51: Blunt-body flow; $u_\infty = 5.5$ km/s, $r = 2.54$ cm, $\rho_\infty = 5.5 \times 10^{-3}$ kg/m$^3$, $T_\infty = 1,400$ K.
Predicted constant density contours.
Figure 6.52: Blunt-body flow; $u_\infty = 5.5 \text{ km/s}$, $r = 2.54 \text{ cm}$, 
$\rho_\infty = 5.5 \times 10^{-3} \text{ kg/m}^3$, $T_\infty = 1,400 \text{ K}$.
Predicted stagnation streamline temperature.

Figure 6.53: Blunt-body flow; $u_\infty = 5.5 \text{ km/s}$, $r = 2.54 \text{ cm}$, 
$\rho_\infty = 5.5 \times 10^{-3} \text{ kg/m}^3$, $T_\infty = 1,400 \text{ K}$.
Solution convergence.
Chapter 7

Numerical Results for Implicit Multigrid Method

7.1 Introductory Remarks

The performance of the proposed partially-decoupled implicit multigrid TVD algorithm of Chapter 5 for predicting steady thermochemical nonequilibrium flows is now assessed by considering some further numerical results for the three two-dimensional stationary flow problems of Chapter 6. They are: 1) the supersonic nozzle flow of air; 2) the compression ramp flow of air; and 3) the blunt-body flow of nitrogen. The five-species four-temperature thermodynamic model of Appendix C is again used in all of the computations. Some earlier results similar to these have been presented by Groth and Gottlieb [1992].

7.2 Numerical Results and Discussion

7.2.1 Supersonic Nozzle Flow of Air

Consider first the steady supersonic diverging nozzle flow problem of Section 6.5.1. The numerical predictions of the fully implicit algorithm for this test case are shown in Figures 6.38 and 6.40 of Chapter 6.

In order to assess the effectiveness of the implicit multigrid method, a higher-order single-grid solution to this problem was first computed using the factored fully implicit partially-decoupled TVD scheme and the 64 × 32 grid shown in Figure 6.37. In this case, Θ = 1, Ω = 0, θ = 0, and β = 1, and a CFL number of unity was employed. A uniform freestream was assumed for the initial data and 800–900 iterations (time steps) were performed before the solution residual, \( \epsilon = \sum_i |\Delta \rho_i|/(N_p \rho_i) \), was reduced by three to four orders of magnitude. The diverging nozzle flow problem was then computed using the implicit algorithm in conjunction with the four-level V-cycle multigrid procedure of Chapter 5. Two pre-smoothing iterations were carried out at each level and the three coarse grids used in the calculations were 32 × 16, 16 × 8, and 8 × 4, respectively. The FMG strategy was invoked.

Both the single-grid and multigrid solutions obtained from the preceding computations are virtually indistinguishable from the previous single-grid results presented in Section 6.5.1 of Chapter 6. Accordingly, plots of these two numerical solutions are not shown. Instead, the convergence rates (i.e., residual reduction rates) of the single-grid and multigrid calculations are of primary interest. In order to compare, in a meaningful way, the convergence rates of these two solutions, the central-processing-unit (CPU) times of both calculations were recorded and then used to determine the convergence as a function of normalized com-
putational work units (i.e., CPU time). The resulting convergence histories of the single-grid and multigrid computations are given in Figure 7.1. It can be observed from the figure that the multigrid method is able to enhance somewhat the steady-state convergence rate for this problem, particularly early in the calculation. The multigrid method would appear to increase the solution convergence by a factor of between two and three. Note that peaks in the convergence history curve of the multigrid computation are associated with the grid transfers of the FMG procedure.

7.2.2 Blunt-Body Flow in Nitrogen, $M_{\infty} = 6.9$

The blunt-body flow problem of Section 6.5.3 is also reconsidered in the multigrid method appraisal. A higher-order accurate single-grid solution to this flow problem was again computed using the implicit TVD scheme and the $96 \times 96$ grid of Figure 6.49. Uniform free-stream initial data were used and the computations were carried out until the residual $\epsilon$ was reduced by about three orders of magnitude. This required some 2,500 iterations with a CFL number of 2. A corresponding solution to this problem was also determined by employing the four-level V-cycle FAS multigrid algorithm of Chapter 5. The $96 \times 96$ grid of Figure 6.49 was used as the fine grid and the associated coarse grids were $48 \times 48$, $24 \times 24$, and $12 \times 12$. These approximate single-grid and multigrid solutions are identical to the result of Figures 6.51 and 6.52 and are therefore not shown.

The convergence history of the multigrid solution for the blunt-body flow problem is depicted in Figure 7.2, again, as a function of computational work units. Also shown in the figure is the associated single-grid convergence behavior. For this problem, it is quite evident that the multigrid method offers significant gains. The multigrid procedure increases the nonequilibrium flow solution convergence by a factor of at least four.

7.2.3 Compression Ramp Flow in Air, $M_{\infty} = 22$

The last problem studied in the assessment of the proposed multigrid method for stationary thermochemical nonequilibrium flows is the oblique shock reflection flow of air at a compression ramp with a free-stream Mach number of $M_{\infty} = 22$ and a wedge angle of $20^\circ$. This problem was also considered in Chapter 6. Refer to Section 6.5.2 for further details.

A higher-order accurate single-grid solution to this problem was computed using the factored fully implicit partially-decoupled TVD scheme on a $96 \times 40$ grid. A uniform free-stream was assumed for the initial data and about 350 iterations were required to reduce the solution residual measure, $\epsilon = \sum_i |\Delta \rho_i|/(N_p \rho_i)$, by four orders of magnitude and to achieve the steady-state result. A CFL number near unity was utilized. The compression ramp flow was also computed using the implicit algorithm in conjunction with the four-level V-cycle multigrid procedure. The three coarse grids used were $48 \times 20$, $24 \times 10$, and $12 \times 5$.

Multigrid convergence rates for both first- and higher-order upwind schemes on the fine grid are shown in Figure 7.3 and compared to the single-grid result. In both cases, the convergence behaviour of the multigrid solutions is poor. The solution converges slowly, more slowly, in fact, than the single-grid solution. This problem was investigated in a previous study by Slomski et al. [1990] using a thermal equilibrium chemical nonequilibrium model. Poor convergence behaviour was also noted therein for this problem. It is felt that the slow convergence rate of the proposed implicit multigrid scheme, and indeed the multigrid method used by Slomski et al., can be attributed to strong grid alignment [Mulder, 1989; Mulder, 1992; Radespiel and Swanson, 1991].
The curvilinear coordinate lines of the grid used in the present computations closely follow the hypersonic flow streamlines. For inviscid flow computations like this, in which grid lines are aligned with the flow direction, multigrid techniques can fail to converge. As discussed in Chapter 5, it is now quite well known that the desirable convergence rates of multigrid methods can be severely reduced for inviscid flow problems in which the lines of the computational mesh are strongly aligned with the flow streamlines. For these cases, Mulder [1988; 1989] has shown that grid-point decoupling occurs in the direction normal to the flow. High-frequency errors are therefore not eliminated on the fine mesh, and, consequently, convergence rates deteriorate. The ramp flow problem was considered herein specifically to investigate the performance of the proposed multigrid method for problems with grid alignment. The convergence histories of Figure 7.3 would indicate that the method is hampered by alignment problems. One possible remedy would be the use of a semi-coarsening technique [Mulder, 1989; Mulder, 1992; Radespiel and Swanson, 1991]. It is important to note that grid alignment is not an issue for viscous flows.

7.3 Summary of Numerical Results

In summary, although convergence of the implicit multigrid TVD scheme is found to be slow for problems with strong grid alignment (i.e., the method suffers from grid alignment problems), this preliminary investigation has provided some encouraging results. It has shown that the proposed multigrid method is potentially useful for thermochemical nonequilibrium flow applications. For the blunt-body flow, computational times for the method are up to factors of four less than those for a single grid procedure. Nevertheless, it should be emphasized that these results are preliminary. The limitations of the available computational resources (i.e., Hewlett-Packard/Apollo 400s workstations) has meant that the residuals in most of the calculations described above have only been reduced by about three orders of magnitude. Although it can be argued that this is usually sufficient for engineering accuracy [Turkel et al., 1991], it was felt that further investigation of the method is required before any strong conclusions can be drawn.
Figure 7.1: Supersonic diverging nozzle flow; $M_e = 1.5$, $y/y_e = 9.1$, $p_e = 101.325$ kPa, $T_e = 6,000$ K. Multigrid solution convergence.

Figure 7.2: Blunt-body flow; $u_\infty = 5.5$ km/s, $r = 2.54$ cm, $\rho_\infty = 5.5 \times 10^{-3}$ kg/m$^3$, $T_\infty = 1,400$ K. Multigrid solution convergence.
Figure 7.3: Compression ramp flow; $M_\infty = 22$, $\theta = 20^\circ$, $p_\infty = 0.21997$ kPa, $T_\infty = 255.88$ K. Multigrid solution convergence.
Chapter 8
Concluding Discussion

8.1 Summary and Conclusions

Recent interest in advanced transportation systems capable of high-speed re-entry and/or transatmospheric flight has fostered renewed research activity in all areas of hypersonic aerodynamics. Computational fluid dynamics is a particularly important design tool for these hypersonic transport and re-entry vehicles. However, unlike subsonic, transonic, and supersonic flow regimes, the physical chemistry associated with the hypersonic flow regimes can be very complex. The presence of strong normal and oblique shock waves in the stagnation regions of hypersonic flows and the extreme viscous dissipation that occurs within hypersonic boundary layers can create very high temperatures. Nonequilibrium finite-rate thermochemical effects such as vibrational relaxation, dissociation, and recombination can become very important. To predict flows predominated by strong shock waves and thermal and chemical nonequilibrium processes, accurate, robust, and efficient CFD algorithms must be devised to solve large systems of conservation laws with often stiff inhomogeneous source terms.

The advent of modern nonlinear shock-capturing techniques has provided the means by which higher-order monotonic oscillation-free solutions of multidimensional gaseous flows with strong discontinuities, such as shock waves, contact surfaces, and slip streams, can be effectively computed. These shock-capturing techniques are therefore appropriate for steady and unsteady hypersonic flow applications; however, extended versions of the algorithms are necessary for the prediction of flows with high-temperature and real-gas phenomena. With this motivation in mind, the goal of the current thesis was to explore the extension of modern upwind TVD finite-difference schemes for the computation of thermochemical nonequilibrium high-temperature flows. The aim was to develop reliable and computationally efficient high-resolution schemes for the numerical solution of high-speed flows characterized by strong shocks and nonequilibrium phenomenon.

To this end, semi-implicit and factored fully implicit extended versions of the upwind-based TVD finite-difference schemes of Roe and Chakravarthy and Osher have been described for predicting steady and unsteady, two-dimensional, inviscid flows in thermal and chemical nonequilibrium. Like other TVD methods, the proposed FDS schemes are smart solution adaptive methods that provide improved numerical accuracy and monotonic or oscillation-free solutions near discontinuities by having solution-dependent difference coefficients. The methods solve the governing hyperbolic conservation laws for vibrationally relaxing and chemically reacting flows of thermally-perfect gaseous mixtures by means
of a partially-decoupled flux-difference splitting approach. The decoupling procedure has been described and algorithm details have been discussed for the resulting frozen-flow gas-dynamic and finite-rate thermodynamic subsystems. This has included a presentation of reformulations of Roe's approximate Riemann solver for the gas-dynamic subsystem, which are essential to performing the flux-difference splitting (see Appendix A), as well as various wavespeed corrections necessary for obtaining physically realistic solutions. The partially-decoupled approach would appear to offer many of the computational simplifications and savings of uncoupled or chemistry-split procedures, while affording solution quality comparable to that of fully coupled algorithms (i.e., the solutions are monotonic and positively conservative, as well as preserve the maximum principle of Larrouturou).

Considerable effort has been devoted herein to the verification and validation of the partially-decoupled techniques. This was accomplished by solving a fairly diverse set of nonstationary and stationary gas-dynamic flow problems, which feature complex nonlinear wave interactions and shock structure and/or exhibit substantial vibrational and chemical nonequilibrium effects, and through the careful comparison of numerical results to available experimental data. Numerical computations were presented for nonstationary one-dimensional flows, unsteady oblique shock-wave reflections and diffractions, as well as for steady supersonic nozzle, compression ramp, and blunt body flows. The success of the partially-decoupled approach was demonstrated by these results. Moreover, the proposed semi-implicit and fully implicit TVD schemes were shown to be capable of providing accurate resolution of shocks and to be quite effective in treating relatively large systems of equations with stiff source terms.

Additionally, an implicit multigrid TVD technique for steady inviscid nonequilibrium hypersonic flow prediction has also been proposed and its effectiveness demonstrated. The method utilizes the proposed fully implicit TVD scheme as the smoothing algorithm and thereby provides accurate resolution of shocks and effective treatment of stiff source terms. Although convergence of the method was found to be slow for problems with strong grid alignment, this preliminary study has shown that multigrid is potentially useful for thermochemical nonequilibrium flows. In some cases, computational times for the multigrid method are at least factors of three to four less than those for the equivalent single grid procedure. However, further study is required.

Some secondary contributions of the thesis relate to the application of the proposed solution techniques. In the present study, a number of the high-Mach-number oblique shock reflection Mach-Zehnder interferometric results of Deschambault and Glass were re-interpreted and then carefully compared to new numerical computations obtained by employing the semi-implicit partially-decoupled TVD upwind scheme. All of the cases considered exhibit finite-rate dissociation/recombination and vibrational relaxation effects. Difficulties with the interpretation of the interferograms in these cases were identified and the computation of actual numerical interferograms (iso-intensity distributions) were found to be most suitable for comparing numerical and experimental results. It is felt that this work has improved the interpretation of the interferogram data and furthered the understanding of oblique shock reflection flows.

In another application, a generalized quasi-one-dimensional nonstationary flow analysis and associated TVD solution schemes were developed for predicting high-temperature flows in the UTIAS-RPI hypersonic impulse tunnel (see Appendix B). The analysis was used to investigate the operation of this experimental facility and to produce performance data that are not always easily determined or available from experimental measurements. The thermodynamic state of the nozzle-exit flow and high-temperature and real-gas effects were
assessed under various operating conditions. Numerical results, coupled with additional comparisons with available experimental data, have demonstrated the range of test-section flows that may be achieved.

8.2 Recommendations for Future Work

Although progress has been made in the development of effective numerical techniques for the computation of high-speed thermochemical nonequilibrium flows with strong shock, further study is needed to fully optimize the methods. For instance, it is felt that research is required to examine whether the convergence of the factored implicit algorithm can be significantly improved by employing different linearization procedures for the implicit operators (e.g., conservative linearization techniques), and/or sophisticated preconditioning techniques, or whether unfactored implicit schemes such as point and line relaxation techniques (e.g., [Yee and Shinn, 1989; Gnoffo and McCandless, 1986; Gnoffo et al., 1987; Gnoffo, 1989; Chakravarthy, 1987]) provide steady-state solutions in a more efficient manner. It is also felt that an investigation of solution-adaptive and/or embedded gridding techniques may be beneficial, particularly for the more accurate resolution of discontinuities. In relation to all of this, further appraisal of the multigrid method is also warranted. Future work on extending the proposed schemes for the solution of viscous and ionizing gaseous flows is also possible. The consideration of laminar flows and simple ionization reaction mechanisms would be the appropriate first step in these directions.
Appendix A

Approximate Solutions of Riemann Problems for the Conservation Laws of Gas Dynamics in Generalized Curvilinear Coordinate Space

A.1 Summary

Approximate Riemann solvers for the conservation laws of inviscid compressible gas dynamics in generalized curvilinear coordinate space are presented. The presentation includes the derivation and final results for the cases of polytropic (ideal), real equilibrium, and frozen nonequilibrium gases. The approximate Riemann solutions may be used in conjunction with many modern upwind solution schemes that employ flux-difference splitting approaches to obtain both stationary and nonstationary solutions to the governing flow equations. The theory and derivation of the approximate solvers are described and pertinent equations given. The analysis is restricted to two-dimensional flows, but Riemann solutions for the three-dimensional case readily follow from the two-dimensional results.

A.2 Introduction

Consider the system of hyperbolic conservation laws in one spatial dimension given by

\[
\frac{\partial U}{\partial t} + \frac{\partial}{\partial x}[F(U)] = \frac{\partial U}{\partial t} + A \frac{\partial U}{\partial x} = 0 ,
\]

(A.1)

where \( U \) is the solution vector, which is a function of \( x \) and \( t \), and \( A = \partial F/\partial U \) is the flux Jacobian matrix. The well-known Riemann problem for the system of Eq. (A.1) is an initial value problem (IVP) with simplified two-state piecewise constant initial data

\[
U(x, t = 0) = \begin{cases} 
U_l, & x \leq 0 , \\
U_r, & x > 0 . 
\end{cases}
\]

(A.2)

If the system is strictly hyperbolic (i.e., the eigenvalues of \( A \) are all real), a generalized (weak) solution of the Riemann IVP exists. The weak solution is self-similar (i.e., depends only on \( x/t \)) and consists of a number of constant states separated by centered elementary waves, such as rarefaction waves, shocks, and/or contact discontinuities. The algorithm for determining such a solution shall be referred to as a Riemann solver.

In computational fluid dynamics (CFD) research, Riemann problems and their solutions have proven to be key ingredients in a number of the more successful shock-capturing tech-
niques for solving flows involving strong shocks and discontinuities. Formulas for evaluating the inviscid flux functions of many numerical methods are often derived by exploiting Riemann problem solution information. Godunov [Godunov, 1959; Godunov et al., 1961] was the first to devise a finite-difference of this type. In his first-order explicit method, Riemann problems are solved at computational cell interfaces to obtain the evolving solution changes. Other subsequent schemes also make use of the Riemann problem, such as the rather unique random choice method (RCM) that arose from the theoretical existence proof of Glimm [1965] and the various forms of higher-order Godunov-type methods that have superseded the first-order version [van Leer, 1979; Colella and Woodward, 1984; Ben-Artzi and Falcovitz, 1984; Ben-Artzi, 1989; Toro, 1989]. In addition, Riemann solvers are very often utilized in the application of upwind and symmetric total-variation diminishing (TVD) schemes [Harten, 1983; Harten, 1984; Roe, 1981; Roe and Pike, 1984; Roe, 1984; Davis, 1984; Yee, 1987a; Yee, 1987b; Osher and Chakravarthy, 1984; Chakravarthy and Osher, 1985a; Chakravarthy and Osher, 1985b]. Used in concert with flux-difference splitting or local characteristic decomposition techniques, the solvers provide a means by which TVD schemes, originally developed for scalar conservation laws, can be extended to cope with the vector nature of hyperbolic systems. Note that the flux-vector splitting techniques of Steger and Warming [1981] and van Leer [1982] can also be used for this purpose. However, these techniques are not considered here.

Most of the early compressible flow shock-capturing schemes were developed for the case of a polytropic (ideal) equation of state, and exact (in contrast to approximate) Riemann solvers were employed in many of these methods. For the ideal gas case, exact self-similar solutions to Riemann problems may be determined fairly readily and efficiently using an iterative numerical technique (see, for example, the paper by Gottlieb and Groth [1988]). However, for fluid flows with more general and/or realistic equations of state, an account of which is given by Menikoff and Plohr [1989], the exact solution of the Riemann problem requires considerably more computational effort. Moreover, except for the RCM of Glimm, most numerical methods that utilize the Riemann problem do not require all of the information that results from an exact solution. A reasonable estimate that closely approximates the essential or relevant features of the exact solution is usually sufficient. For these reasons, approximate solvers have been devised and are used quite extensively. These non-exact solvers are usually noniterative and are therefore generally more efficient than exact solution procedures.

Motivated by this desire to reduce computational work associated with Riemann problem solution, a number of approximate methods have been proposed. Acoustic, two-shock, and two-rarefaction wave or isentropic approximations have all been suggested for the ideal gas case (polytropic equation of state) [Godunov et al., 1961; Colella and Glaz, 1985; Dukowicz, 1985; Gottlieb and Groth, 1988; Jacobs, 1992]. For real gases, Colella and Glaz [1985] have developed an approximate but still iterative procedure for constructing solutions to the Riemann problem with a general convex equation of state. In another study, Dukowicz [1985] describes a noniterative two-shock solver for various real materials (solid, liquid, and gas) obeying approximate shock Hugoniotics. Osher has also proposed a two-rarefaction wave approximate solution procedure for the Riemann problem which has recently been extended to include gases with an arbitrary equation of state [Suresh and Liou, 1991]. All of these approximate solutions have merit; however, the linearized approximate solver of Roe [1981] has probably gained the most widespread use within the shock-capturing CFD community. This relatively efficient solver, initially developed for polytropic gases in Cartesian coordinate space, has the rather remarkable and useful feature that it

A.2
produces the exact solution for the case of a single discontinuity. Later work by Glaister has provided extensions to the Roe solver for a general equation of state [Glaister, 1988a; Glaister, 1988b], for a generalized curvilinear (body-fitted) coordinate space [Glaister, 1988d], and for flows with axial symmetry [Glaister, 1988c]. Other researchers have also developed extended Roe-type Riemann solvers for application to flows of real gases with equilibrium and nonequilibrium thermodynamics and/or chemistry [Vinokur and Liu, 1988; Grossman and Walters, 1989; Liu et al., 1990; Liu and Vinokur, 1989; Shuen et al., 1990].

Of interest in this appendix are approximate solutions to the Riemann problem for the Euler equations describing inviscid two-dimensional planar flow of compressible gases. Two cases are considered. The first is the case in which the gas is always in complete thermodynamic equilibrium (thermal and chemical equilibrium) and its behaviour can be represented by an equation of state relating pressure, density, and internal energy. The second is the case in which the gas is a frozen nonequilibrium thermally perfect mixture. For the first case, the extended Roe-type approximate Riemann solvers of Glaister for a generalized curvilinear coordinate space are reviewed. Additional extensions are then given for the frozen nonequilibrium flow case. Included in the presentation are descriptions of the governing flow equations of interest and their eigensystems, as well as a thorough development of the analyses leading to the approximate solutions. The solvers described herein may be used in conjunction with many modern upwind schemes that employ flux-difference splitting approaches to obtain compressible flow solutions.

A.3 Gas Dynamic Conservation Laws

This development of the approximate Riemann solvers commences with the presentation of the gas dynamics conservation laws of interest. The forms of the Euler equations to be considered are expressed in terms of a generalized curvilinear coordinate system.

A.3.1 Euler Equations for a General Equilibrium Equation of State

Confining ourselves to inviscid two-dimensional planar flows, the conservation law forms of mass, momentum, and energy equations for a gas in thermal and chemical equilibrium can be written in vector form as

$$\frac{\partial}{\partial t}(J \mathbf{U}) + \frac{\partial}{\partial \zeta}[\mathbf{F}(\mathbf{U})] + \frac{\partial}{\partial \eta}[\mathbf{G}(\mathbf{U})] = 0,$$

(A.3)

where the four-component solution column vector $\mathbf{U}$ is given by

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho [e + \frac{1}{2} (u^2 + v^2)] \end{bmatrix},$$

(A.4)

and the flux column vectors $\mathbf{F}$ and $\mathbf{G}$ are

$$\mathbf{F} = \begin{bmatrix} \rho \mathbf{U} \\ \rho u \mathbf{U} + \gamma \rho p \\ \rho v \mathbf{U} - x \rho p \\ \rho \mathbf{U} \left[ e + \frac{p}{\rho} + \frac{1}{2} (u^2 + v^2) \right] \end{bmatrix}, \quad \mathbf{G} = \begin{bmatrix} \rho \mathbf{V} \\ \rho \mathbf{V} - \gamma \rho p \\ \rho \mathbf{V} + x \rho p \\ \rho \mathbf{V} \left[ e + \frac{p}{\rho} + \frac{1}{2} (u^2 + v^2) \right] \end{bmatrix}.$$

(A.5)
In Eqs. (A.3)-(A.5), \( t \) is time, \( x \) and \( y \) are the Cartesian coordinates of the physical space, \( \rho \) is the density, \( u \) and \( v \) and the velocity components in the physical coordinate system, \( e \) is the specific internal energy, and \( p \) is the pressure. The variables \( \zeta \) and \( \eta \) are the curvilinear coordinates of the transformed or computational space, \( x_\zeta = \partial x / \partial \zeta \), \( x_\eta = \partial x / \partial \eta \), \( y_\zeta = \partial y / \partial \zeta \), \( y_\eta = \partial y / \partial \eta \) are the metrics of the coordinate transformation \( x = x(\zeta, \eta) \), \( y = y(\zeta, \eta) \), and \( J = x_\zeta y_\eta - x_\eta y_\zeta \) is the transformation Jacobian. \( U = y_\eta u - x_\eta v \) and \( V = x_\zeta v - y_\zeta u \) are the contravariant velocities. Note that a brief discussion of generalized curvilinear coordinates is given in Appendix D.

The preceding system of equations is cast in strong conservation law form. Closure of the system is obtained via an equation of state (EOS) which relates the pressure to the other state variables. In the present analysis, the EOS is assumed to have the form

\[ p = p(\rho, e) \tag{A.6} \]

It is further assumed that the function \( p(\cdot, \cdot) \) satisfies conditions which guarantee that the system of Eq. (A.3) is strictly hyperbolic and that unique solutions exist to the corresponding Riemann problems for this system with initial data of the form given by Eq. (A.2). Note that the inequalities \( \partial p / \partial \rho > 0 \) and \( \partial p / \partial e > 0 \) are sufficient but not necessary conditions for ensuring that Eq. (A.3)–(A.5) possess these features [Colella and Glaz, 1985; Smith, 1979]. Note also that in the case of a polytropic (thermally and calorically perfect) gas, the pressure \( p \) is given by the ideal-gas EOS which can be written as

\[ p = (\gamma - 1)\rho e = \rho R T \tag{A.7} \]

where \( \gamma \) is the specific heat ratio of the gas, \( R \) is the gas constant, and \( T \) is the temperature.

### A.3.2 Euler Equations for a Frozen Thermally Perfect Mixture

The other system of hyperbolic conservation laws that is of concern here is the set of PDEs describing the inviscid flow of a thermally and chemically frozen mixture of thermally perfect gases for which the mixture thermal state is described by a translational-rotational temperature and a set of vibrational temperatures, one for each molecular species. The governing conservation laws for the mixture, once again expressed in terms of a generalized two-dimensional curvilinear coordinate system, may be written as

\[ \frac{\partial}{\partial t}(JU) + \frac{\partial}{\partial \zeta}[F(U)] + \frac{\partial}{\partial \eta}[G(U)] = 0 \tag{A.8} \]

where the solution and flux column vectors are

\[ U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho \left[ \frac{p}{\gamma - 1} + e_v + \frac{1}{2}(u^2 + v^2) \right] \\ \rho \gamma \\ \rho R \\ \rho e_v \end{bmatrix} \tag{A.9} \]
and where $\rho$, $u$, $v$, $p$, $e_v$, $\gamma$, and $R$ are the mixture density, velocity components, pressure, specific vibrational energy, specific heat ratio, and gas constant, respectively. The mixture pressure may be related to the density and translational-rotational temperature $T$ or specific translational-rotational energy $e_{tr}$ by the EOS $p = \rho RT = (\gamma - 1)\rho e_{tr}$.

The seven-component system of Eqs. (A.8)-(A.10) can be derived from a complete set of thermochemical nonequilibrium flow equations, which include finite-rate inhomogeneous source terms, by employing a frozen-flow assumption. The resulting frozen-flow equations describe the nonequilibrium gaseous flow in the limit as the Damköhler number approaches zero. The behaviour of the mixture is essentially that of a polytropic gas, except that the specific heat ratio and gas constant may vary throughout the flow field and a portion of the internal energy is locked in the vibrational modes. The last three PDEs of Eqs. (A.8)-(A.10) are introduced to include these effects and describe changes in the quantities $\gamma$, $R$, and $e_v$, that, in the frozen flow limit, are merely convected with the flow.

### A.4 Eigenvalues and Eigenvectors of Flux Jacobians

The approximate Riemann problem solution procedure of Roe requires information about the eigensystems of the flux Jacobians for the particular hyperbolic system under consideration. For the preceding conservation laws, the eigenvectors and eigenvalues of the flux Jacobians $A = \partial F/\partial U$ and $B = \partial G/\partial U$ are needed and are therefore derived below.

#### A.4.1 Eigensystems for a General Equilibrium Equation of State

For the equilibrium flow equations, the $\zeta$-direction flux Jacobian matrix $A = \partial F/\partial U$ can be written as

$$A = \begin{bmatrix}
0 & y_\eta & -x_\eta & 0 \\
y_\eta \left[ a^2 - \frac{1}{\rho} \frac{\partial \rho}{\partial e} (h - u^2 - v^2) \right] - uU & U + y_\eta u \left( 1 - \frac{1}{\rho} \frac{\partial \rho}{\partial e} \right) & -x_\eta u - y_\eta \frac{v \frac{\partial \rho}{\partial e}}{\rho} & \frac{y_\eta \frac{v \frac{\partial \rho}{\partial e}}{\rho}}{\rho} \\
-x_\eta \left[ a^2 - \frac{1}{\rho} \frac{\partial \rho}{\partial e} (h - u^2 - v^2) \right] - vU & y_\eta \nu + x_\eta \frac{\partial \nu}{\partial \rho} & U - x_\eta \nu \left( 1 - \frac{1}{\rho} \frac{\partial \rho}{\partial e} \right) & -x_\eta \nu \frac{U \frac{\partial \rho}{\partial e}}{\rho} \\
U \left( a^2 - h \right) - \frac{U \frac{\partial \rho}{\partial e} (h - u^2 - v^2)}{\rho} & y_\eta h - \frac{U \frac{\partial \rho}{\partial e}}{\rho} & -x_\eta h - \frac{vU \frac{\partial \rho}{\partial e}}{\rho} & U + \frac{U \frac{\partial \rho}{\partial e}}{\rho} \\
\end{bmatrix}, \quad (A.11)$$

\[1\] The Damköhler number is defined to be the ratio of the convection or advection time scale to the time scales associated with the thermochemical processes [Oran and Boris, 1987].

A.5
for which the variable $a$ is the sound speed of the gas defined by the relationship

$$a^2 = \frac{\partial p}{\partial \rho} = \frac{\partial p}{\partial \rho} + \frac{p}{\rho^2} \frac{\partial p}{\partial \rho},$$

(A.12)

where $s$ is the entropy. The quantity $h = e + p/\rho + (u^2 + v^2)/2$ appearing in Eq. (A.11) is the specific enthalpy of the gas. It can be shown that $a^2 = \gamma p/\rho = \gamma RT$ for the case of a polytropic gas.

The four eigenvalues $\lambda_k$ and right eigenvectors $e_k$ of the $4 \times 4$ $\zeta$-direction flux Jacobian matrix can be determined by considering the eigenvalue problem $\mathbf{A}e_k = \lambda_k e_k$, for $k = 1, \ldots, 4$. The resulting eigenvalues are

$$\lambda_1 = U - a\sqrt{x_n^2 + y_n^2}, \quad \lambda_2 = \lambda_3 = y_nu - x_nv = U, \quad \lambda_4 = U + a\sqrt{x_n^2 + y_n^2},$$

(A.13)

and the corresponding eigenvectors are

$$e_1 = \begin{bmatrix} 1 \\ u - \frac{y_n a}{\sqrt{x_n^2 + y_n^2}} \\ v + \frac{x_n a}{\sqrt{x_n^2 + y_n^2}} \\ h - \frac{a U}{\sqrt{x_n^2 + y_n^2}} \end{bmatrix}, \quad e_4 = \begin{bmatrix} 1 \\ u + \frac{y_n a}{\sqrt{x_n^2 + y_n^2}} \\ v - \frac{x_n a}{\sqrt{x_n^2 + y_n^2}} \\ h + \frac{a U}{\sqrt{x_n^2 + y_n^2}} \end{bmatrix},$$

(A.14)

$$e_2 = \begin{bmatrix} 1 \\ u \\ v \\ h - \frac{\rho}{\partial p} \frac{\partial p}{\partial e} \end{bmatrix}, \quad e_3 = \begin{bmatrix} 0 \\ x_n \\ y_n \\ x_n u + y_n v \end{bmatrix},$$

(A.15)

Again, for the special case of a polytropic or perfect gas, $\partial p/\partial e = (\gamma - 1)p$ and, therefore, $h - \rho a^2/(\partial p/\partial e) = (u^2 + v^2)/2$. Note that because the conservation laws are strictly hyperbolic, the sound speed $a$ is real and the flux Jacobian $\mathbf{A}$ has a complete set of real-valued eigenvalues.

Similar results can be obtained for the $\eta$-direction flux Jacobian $\mathbf{B} = \partial \mathbf{G}/\partial \mathbf{U}$. Application of the chain rule results in the following expression for this Jacobian matrix:

A.6
and the associated eigenvalues and eigenvectors that satisfy $\mathbf{B} \mathbf{e}_k = \lambda_k \mathbf{e}_k$ are then

$$
\lambda_1 = V - a \sqrt{x_\zeta^2 + y_\zeta^2}, \quad \lambda_2 = \lambda_3 = x_\zeta v - y_\zeta u = V, \quad \lambda_7 = V + a \sqrt{x_\zeta^2 + y_\zeta^2},
$$

$$(A.17)$$

$$
\mathbf{e}_1 = \begin{bmatrix} 1 \\ u + \frac{y_\zeta a}{\sqrt{x_\zeta^2 + y_\zeta^2}} \\ v - \frac{x_\zeta a}{\sqrt{x_\zeta^2 + y_\zeta^2}} \\ h - \frac{a V}{\sqrt{x_\zeta^2 + y_\zeta^2}} \end{bmatrix}, \quad \mathbf{e}_4 = \begin{bmatrix} 1 \\ u - \frac{y_\zeta a}{\sqrt{x_\zeta^2 + y_\zeta^2}} \\ v + \frac{x_\zeta a}{\sqrt{x_\zeta^2 + y_\zeta^2}} \\ h + \frac{a V}{\sqrt{x_\zeta^2 + y_\zeta^2}} \end{bmatrix},
$$

$$(A.18)$$

$$
\mathbf{e}_2 = \begin{bmatrix} 1 \\ u \\ v \\ h - \frac{\rho}{\partial p/\partial e} \end{bmatrix}, \quad \mathbf{e}_3 = \begin{bmatrix} 0 \\ x_\zeta \\ y_\zeta \\ x_\zeta u + y_\zeta v \end{bmatrix}.
$$

$$(A.19)$$

It is worth noting that $\mathbf{A}$ and $\mathbf{B}$ each have only three distinct eigenvalues; however four distinct eigenvectors may be identified. The $k = 1$ and 4 characteristic fields of both matrices are genuinely nonlinear in the sense of Lax [1973] (i.e., $\partial \lambda_k/\partial \mathbf{U} \cdot \mathbf{e}_k \neq 0$), whereas the $k = 2$ and 3 eigenvalues and eigenvectors are linearly degenerate and are associated with purely convective fluxes.

### A.4.2 Eigensystems for a Frozen Thermally Perfect Mixture

The flux Jacobian eigensystems for the conservation laws of the thermally and chemically frozen nonequilibrium gaseous mixture can be derived in an identical manner. However, in this case, the eigensystems are somewhat larger. The $7 \times 7 \zeta$-direction flux Jacobian matrix $\mathbf{A} = \partial \mathbf{F}/\partial \mathbf{U}$ is given by
and the eigenvalues $\lambda_k$ and eigenvectors $e_k$ satisfying $A e_k = \lambda_k e_k$ for $k = 1, \ldots, 7$ are

$$\begin{align*}
\lambda_1 &= U - a \sqrt{x_n^2 + y_n^2}, \quad \lambda_7 = U + a \sqrt{x_n^2 + y_n^2}, \\
\lambda_2 &= \lambda_3 = \lambda_4 = \lambda_5 = \lambda_6 = y_n u - x_n v = U,
\end{align*}$$

(A.21)

(A.22)
In Eqs. (A.20)-(A.24), \( a \) is the frozen sound speed for the mixture that may be related to the other intensive properties by the expression

\[
a^2 = \frac{\gamma p}{\rho} = \gamma (\gamma - 1) e_{tr} = \gamma RT, \tag{A.25}
\]

and \( h \) is the specific enthalpy of the mixture defined by

\[
h = e_{tr} + \frac{p}{\rho} + \gamma v + \frac{1}{2}(u^2 + v^2) = \frac{\gamma p}{(\gamma - 1)\rho} + \gamma v + \frac{1}{2}(u^2 + v^2). \tag{A.26}
\]

A similar expression to that of Eq. (A.20) may be obtained for the \( \eta \)-direction flux Jacobian matrix \( B = \partial G / \partial U \) and a subsequent analysis of the eigenvalue problem \( B e_k = \lambda_k e_k \) yields the following eigenvalues and eigenvectors:

\[
\lambda_1 = V - a \sqrt{x_\eta^2 + y_\eta^2}, \quad \lambda_7 = V + a \sqrt{x_\eta^2 + y_\eta^2}, \tag{A.27}
\]

\[
\lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = \lambda_6 = x_\zeta v - y_\zeta u = V, \tag{A.28}
\]

\[
e_1 = \begin{bmatrix} u - \frac{y_\eta a}{\sqrt{x_\eta^2 + y_\eta^2}} \\ v + \frac{x_\eta a}{\sqrt{x_\eta^2 + y_\eta^2}} \\ h - \frac{a U}{\sqrt{x_\eta^2 + y_\eta^2}} \\ \gamma \\ R \\ e_v \end{bmatrix}, \quad e_2 = \begin{bmatrix} e_v + \frac{1}{2}(u^2 + v^2) \\ \gamma \\ R \\ e_v \end{bmatrix}, \quad e_7 = \begin{bmatrix} u + \frac{y_\eta a}{\sqrt{x_\eta^2 + y_\eta^2}} \\ v - \frac{x_\eta a}{\sqrt{x_\eta^2 + y_\eta^2}} \\ h + \frac{a U}{\sqrt{x_\eta^2 + y_\eta^2}} \\ \gamma \\ R \\ e_v \end{bmatrix}, \tag{A.29}
\]
Observe that, as was the case for the PDEs describing the flow of an equilibrium gas, the flux Jacobians $A$ and $B$ again each have only three distinct eigenvalues.

### A.5 Riemann Problems and Approximate Solutions

The Roe-type approximate Riemann solvers for the aforementioned systems of equations are presented in this section. Although there is ongoing research on multidimensional approximate Riemann solvers and associated multidimensional solution schemes [Roe, 1986b; Powell et al., 1990], most commonly used shock-capturing methods make use of some form of dimensional splitting. Consequently, in the present analysis, Riemann problem solutions are sought for one-dimensional analogues of the given two-dimensional hyperbolic conservation laws. The one-dimensional equation sets correspond to the invariant $\eta$- and $\zeta$-coordinate directions and are given by

$$\frac{\partial}{\partial t} (JU) + \frac{\partial}{\partial \zeta} [F(U)] = 0, \quad \frac{\partial}{\partial t} (JU) + \frac{\partial}{\partial \eta} [G(U)] = 0. \quad (A.31)$$

#### A.5.1 Riemann Solvers for a General Equilibrium Equation of State

Consider first the approximate Riemann solvers for the case of a general equilibrium equation of state. Following Roe [Roe, 1981; Roe and Pike, 1984], solutions to linearized Riemann IVPs for the systems of Eq. (A.31) are sought. In the $\zeta$-direction, the linearized Riemann problems posed about locations $(0,1_0)$ are assumed to have the form

$$\frac{\partial U}{\partial t} + \frac{1}{J_*} A_*(U_*) \frac{\partial U}{\partial \zeta} = 0, \quad t > 0, \quad (A.32)$$

$$U(\zeta, \eta_0, t = 0) = \begin{cases} U_l, & \zeta \leq \zeta_0, \\ U_r, & \zeta > \zeta_0, \end{cases} \quad (A.33)$$

where, as part of the linearization process, the flux Jacobian $A$ of Eq. (A.11) is approximated by a locally constant matrix $A_*$ that depends on a local average state $U_*$. Here, the subscript $*$ denotes an average state. Similarly, $J_*$ is a corresponding local average value for the coordinate transformation Jacobian $J$. The local average state $U_*$ is taken to be a function of the neighboring left and right states $U_l$ and $U_r$ and, in the generalized form of the solver, the left and right states are permitted to be widely different. The motivation for this particular form of linearized Riemann problem stems directly from a desire to employ scalar TVD schemes for the solution of nonlinear systems. In the case of linear systems, the flux Jacobian matrix $A$ is, by definition, a constant coefficient matrix. Therefore, the
system of linear equations can be decoupled into a set of scalar equations by means of a diagonalization procedure. TVD solution algorithms can then be applied independently to each scalar equation in a straightforward manner. For the nonlinear case, a similar procedure can be used if an appropriate locally-frozen constant-coefficient flux Jacobian matrix can be identified. The determination of this mean value Jacobian for the nonlinear case is essentially the aim of the Roe solver.

Like its exact counterpart, for \( t > 0 \), the solution of the linearized Riemann IVP defined by Eqs. (A.32) and (A.33) is self-similar and depends on \( \zeta/t \) only. However, unlike the exact solution which, for the Euler equations of gas dynamics, consists of the usual shocks, contact surfaces, and/or centered rarefaction waves, the left and right states of the approximate solution are assumed to be separated by a self-similar wave pattern composed of several elemental waves and intermediate states. In the present case of the two-dimensional Euler equations for a thermal and chemical equilibrium gas, there are four elemental waves and two intermediate states. See Figure A.1. The speed of each elemental wave is taken to be \( \lambda_{e_k}/J_e \) and the solution jumps across each wave are given by

\[
\Delta U_k = \alpha_{e_k} e_{e_k}, \tag{A.34}
\]

for \( k = 1, 2, 3, \) and \( 4 \). The eigenvalues \( \lambda_{e_k} \) and eigenvectors \( e_{e_k} \) of the flux Jacobian given by Eqs. (A.13)–(A.15) are evaluated at \( U_* \) and \( \alpha_{e_k} \) is the strength of the elemental wave. The task of the approximate Riemann solver is to specify the average state \( U_* \), wave speeds \( \lambda_{e_k} \), and wave strengths \( \alpha_{e_k} \) and thus prescribe the two intermediate solution states between elemental waves 1 and 2 and elemental waves 3 and 4, respectively.

Various average states, and hence, approximate solutions may be defined; however, the appropriate approximate Jacobians \( A_* \) are required to have the following properties:

(i) \( A_* = A(U = U_*) \);

(ii) \( \lim_{U_l - U_r \to U_*} A_* = A \);

(iii) the eigenvectors of \( A_* \) are linearly independent;

(iv) \( \Delta U_{rl} = U_r - U_l = \sum_k \alpha_{e_k} e_{e_k} \); and

(v) \( \Delta F_{rl} = F(U_r) - F(U_l) = F_r - F_l = \sum_k \alpha_{e_k} \lambda_{e_k} e_{e_k} \).

By using these properties, Roe [Roe, 1981; Roe and Pike, 1984] has constructed approximate solutions to Riemann problems for inviscid flows of polytropic gases in Cartesian coordinates and has demonstrated that the aforementioned properties guarantee conservation and afford the associated difference schemes excellent shock-capturing attributes. The last property ensures that the approximate Riemann solution is exact for the case of a single discontinuity in Cartesian coordinates. Among others, Glaister [1988a; 1988b; 1988d] has since extended these ideas for the treatment of the conservation laws describing equilibrium ideal- and real-gas flows in generalized transformed coordinates. Glaister’s results are now reviewed.

By assuming that linearized approximations such as \( \Delta(\rho u)_{rl} = \rho_* \Delta u_{rl} + u_* \Delta \rho_{rl} \) apply in the more general case where the solution jumps are large, the changes in the conserved
Combining this expression with the condition $\Delta U_{rl} = \sum \alpha_{nk} e_{nk}$ (here the eigenvectors act as a set of basis vectors for prescribing solution changes), it is possible to relate the elemental wave strengths to the average state values of the primitive variables $\rho_*, u_*, v_*, e_*, p_*, a_*$, and $h_*$, and solution jumps $\Delta \rho_{rl} = \rho_r - \rho_l$, $\Delta u_{rl} = u_r - u_l$, $\Delta v_{rl} = v_r - v_l$, $\Delta e_{rl} = e_r - e_l$, and $\Delta p_{rl} = p_r - p_l$. The resulting expressions are

$$\alpha_{n1} = \frac{1}{2a_*^2} \left[ \Delta p_{rl} - \rho_* a_* \frac{(y_{n1} \Delta u_{rl} - x_{n1} \Delta v_{rl})}{\sqrt{x_{n1}^2 + y_{n1}^2}} \right], \quad \alpha_{n2} = \Delta \rho_{rl} - \frac{\Delta p_{rl}}{a_*^2}, \quad (A.36)$$

$$\alpha_{n3} = \rho_* \frac{x_{n1} \Delta u_{rl} + y_{n1} \Delta v_{rl}}{(x_{n1}^2 + y_{n1}^2)}, \quad \alpha_{n4} = \frac{1}{2a_*^2} \left[ \Delta p_{rl} + \rho_* a_* \frac{(y_{n1} \Delta u_{rl} - x_{n1} \Delta v_{rl})}{\sqrt{x_{n1}^2 + y_{n1}^2}} \right], \quad (A.37)$$

where $x_{n1}$ and $y_{n1}$ denote local averages of the transformation metrics. Having obtained the wave strengths, the appropriate average state values of the primitive variables $\rho_*, u_*, v_*, e_*$, $p_*$, $a_*$, and $h_*$ can then be determined by employing equations Eqs. (A.36) and (A.37) and by enforcing the condition $\Delta F_{rl} = \sum \alpha_{nk} \lambda_{nk} e_{nk}$. For polytropic gases obeying the ideal EOS, the solution of this system of algebraic equations produces the following averages:

$$\rho_* = \sqrt{\rho r \rho l}, \quad (A.38)$$

$$Z_* = \frac{\sqrt{\rho r Z r} + \sqrt{\rho l Z l}}{\sqrt{\rho r} + \sqrt{\rho l}}, \quad Z = u, v, e, and h, \quad (A.39)$$

$$a_*^2 = (\gamma - 1) \left[ h_* - \frac{1}{2} (u_*^2 + v_*^2) \right], \quad p_* = \rho_* \left[ h_* - e_* - \frac{1}{2} (u_*^2 + v_*^2) \right]. \quad (A.40)$$

For a more general EOS of the form $p = p(\rho, e)$, the preceding averages for $\rho$, $u$, $v$, $e$, $p$, and $h$, are still applicable, but additional relations are required for determining local average-state values for the partial derivatives of the pressure with respect to the density and internal energy and for evaluating an average-state sound speed. In the extended approximate solver of Glaister, the proposed averages for $\partial p/\partial \rho$ and $\partial p/\partial e$ are

$$\frac{\partial p}{\partial \rho}_* = \begin{cases} \frac{1}{2\Delta \rho_{rl}} \left[ (p(\rho_r, e_r) + p(\rho_l, e_l)) - (p(\rho_l, e_r) + p(\rho_l, e_l)) \right] & \Delta \rho_{rl} \neq 0, \\ \frac{1}{2} \left( \frac{\partial p}{\partial \rho_r} + \frac{\partial p}{\partial \rho_l} \right) & \Delta \rho_{rl} = 0, \end{cases} \quad (A.41)$$

$$\frac{\partial p}{\partial e}_* = \begin{cases} \frac{1}{2\Delta e_{rl}} \left[ (p(\rho_r, e_r) + p(\rho_l, e_r)) - (p(\rho_r, e_l) + p(\rho_l, e_l)) \right] & \Delta e_{rl} \neq 0, \\ \frac{1}{2} \left( \frac{\partial p}{\partial e_r} + \frac{\partial p}{\partial e_l} \right) & \Delta e_{rl} = 0, \end{cases} \quad (A.42)$$
and \( a \) is then specified by the expression

\[
a_* = \left( \frac{\partial p}{\partial \rho} + \frac{p_*}{\rho_*^2} \frac{\partial \rho}{\partial \epsilon} \right)^{1/2}.
\]  

(A.43)

The choice of averages for the derivatives of the pressure does not appear to be uniquely defined [Tourni, 1992]. Although other averages have been proposed for the derivatives of the pressure (see, for example, Liou et al. [1990]), it has been demonstrated that this choice of averaging provides accurate solutions in a relatively efficient manner.

Equations (A.36)-(A.43), in combination with the solution and flux jump relations 

\[
\Delta U_{rl} = \sum \alpha_{*k} e_{*k} \quad \text{and} \quad \Delta F_{rl} = \sum \alpha_{*k} \lambda_{*k} e_{*k},
\]

constitute the approximate Riemann solver for the IVP of Eqs. (A.32) and (A.33). The locally constant or approximate Jacobian is given by \( A_* = A(U = U_*) \). It should be emphasized that the left and right states \( U_1 \) and \( U_r \) of the Riemann problem are permitted to be widely different and, for a polytropic gas and cartesian coordinates, the approximate solver returns the exact solution in the case of a single discontinuity.

Solutions to the linearized Riemann problems in the \( \eta \)-direction follow in a similar fashion. In this case, the approximate Riemann problems have the form

\[
\frac{\partial U}{\partial t} + \frac{1}{J_*} B_* (U_*) \frac{\partial U}{\partial \eta} = 0, \quad t > 0,
\]

(A.44)

\[
U(\zeta, \eta, t = 0) = \begin{cases} U_l, & \eta < \eta_0, \\ U_r, & \eta > \eta_0, \end{cases}
\]

(A.45)

and the corresponding wave strengths of the solver providing the characteristic decompositions of the solution and flux vectors \( \Delta U_{rl} = \sum \alpha_{*k} e_{*k} \) and \( \Delta F_{rl} = \sum \alpha_{*k} \lambda_{*k} e_{*k} \) are

\[
\alpha_{*1} = \frac{1}{2a_*^2} \left[ \Delta p_{rl} - \rho_* a_* \left( x_* \Delta v_{rl} - y_* \Delta u_{rl} \right) \right], \quad \alpha_{*2} = \Delta p_{rl} - \frac{\Delta p_{rl}}{a_*^2},
\]

(A.46)

\[
\alpha_{*3} = \rho_* \frac{\left( x_* \Delta u_{rl} + y_* \Delta v_{rl} \right)}{\sqrt{x_*^2 + y_*^2}}, \quad \alpha_{*7} = \frac{1}{2a_*^2} \left[ \Delta p_{rl} + \rho_* a_* \left( x_* \Delta v_{rl} - y_* \Delta u_{rl} \right) \right],
\]

(A.47)

for which the average state primitive variables are again defined by Eqs. (A.38)-(A.43).

### A.5.2 Riemann Solvers for a Frozen Thermally Perfect Mixture

Consider now the approximate Riemann solvers for the case of the frozen thermally perfect mixture. Although the gaseous mixture obeys the ideal EOS, additional extensions to the Roe-type approximate Riemann solvers of Glaister are needed for the frozen-flow case to include the effects of varying \( \gamma \) and \( R \) and non-zero \( e_v \). In the \( \zeta \)-direction, solutions to linearized Riemann IVPs having the form of Eqs. (A.32) and (A.33) are again sought. The solutions are once again self-similar; however, in this case, there are now seven elemental waves \((k = 1, 2, 3, 4, 5, 6, \text{and } 7)\) with wave speeds \( \lambda_{*k} / J_* \) and solution jumps \( \Delta U_k = \alpha_{*k} e_{*k} \). For the frozen thermally perfect mixture, the
jumps in the conserved solution variables $\Delta U_{rl} = U_r - U_l$ can be written as

$$
\Delta U_{rl} = \begin{bmatrix}
\Delta \rho_{rl} \\
\Delta p_{rl} \\
\Delta u_{rl} \rho_{rl} + \Delta \rho_{rl} \\
\Delta v_{rl} \rho_{rl} + \Delta \rho_{rl} \\
\Delta \gamma_{rl} + \rho_{rl} \Delta \rho_{rl} \\
\rho_{rl} \Delta R_{rl} + R_{rl} \Delta \rho_{rl} \\
\rho_{rl} \Delta e_{vrl} + \Delta \rho_{rl}
\end{bmatrix}
$$

(A.48)

Expressions for the elemental wave strengths $\alpha_{*k}$ in terms of the average state values of the primitive variables $\rho_*, u_*, v_*, e_*, p_*, \gamma_*, R_*, e_{v*}, \alpha_*$, and $h_*$, and solution jumps $\Delta \rho_{rl} = \rho_r - \rho_l, \Delta u_{rl} = u_r - u_l, \Delta v_{rl} = v_r - v_l, \Delta p_{rl} = p_r - p_l, \Delta \gamma_{rl} = \gamma_r - \gamma_l, \Delta R_{rl} = R_r - R_l$, and $\Delta e_{vrl} = e_{vr} - e_{vl}$ can then be obtained from Eq. (A.48) and the condition $\Delta U_{rl} = \sum \alpha_{*k} e_{*k}$. The resulting wave strengths are

$$
\alpha_{*1} = \frac{1}{2a_*^2} \left[ \Delta \rho_{rl} - \rho_* a_* \left( y_{*\gamma} \Delta u_{rl} - x_{*\gamma} \Delta v_{rl} \right) \right], \\
\alpha_{*2} = \frac{\Delta \rho_{rl}}{a_*^2}, \\
\alpha_{*3} = \rho_* \frac{(x_{*\gamma} \Delta u_{rl} + y_{*\gamma} \Delta v_{rl})}{(x_{*\gamma}^2 + y_{*\gamma}^2)}, \\
\alpha_{*4} = \frac{p_*}{\gamma_*} \Delta \gamma_{rl}, \\
\alpha_{*5} = \frac{p_*}{R_*} \Delta R_{rl}, \\
\alpha_{*6} = \frac{p_*}{e_{v*}} \Delta e_{vrl}, \\
\alpha_{*7} = \frac{1}{2a_*^2} \left[ \Delta \rho_{rl} + \rho_* a_* \left( y_{*\gamma} \Delta u_{rl} - x_{*\gamma} \Delta v_{rl} \right) \right]
$$

(A.49) - (A.52)

where $x_{*\gamma}$ and $y_{*\gamma}$ again denote local averages of the transformation metrics. The subsequent substitution of these expressions for the waves strengths into $\Delta F_{rl} = \sum \alpha_{*k} \lambda_{*k} e_{*k}$ results in a set of algebraic equations for the appropriate Roe averages of the primitive variables. An appropriate approximate solution of these algebraic equations yields the following averages:

$$
\rho_* = \sqrt{\rho_l \rho_r}, \\
Z_* = \frac{\sqrt{\rho_l} Z_l + \sqrt{\rho_r} Z_l}{\sqrt{\rho_l + \sqrt{\rho_l}}}, \quad Z = u, v, e_{tr}, \gamma_*, R_*, e_{v*}, \text{and } h_*, \\
\alpha_*^2 = (\gamma_* - 1) \left[ h_* - e_{v*} - \frac{1}{2} (u_*^2 + v_*^2) \right], \\
p_* = \rho_* \left[ h_* - e_{tr*} - e_{v*} - \frac{1}{2} (u_*^2 + v_*^2) \right]
$$

(A.53) - (A.55)

and thereby completes the prescription of the Riemann solver for the $\zeta$-direction.

The approximate solver for the linearized Riemann problems in the $\eta$-direction is similar. It can be shown that Eqs. (A.53)-(A.55) again define the desired average state and the wave strengths providing the characteristic decompositions of the solution and flux vectors $\Delta U_{rl} = \sum \alpha_{*k} e_{*k}$ and $\Delta G_{rl} = \sum \alpha_{*k} \lambda_{*k} e_{*k}$ are given by

$$
\alpha_{*1} = \frac{1}{2a_*^2} \left[ \Delta \rho_{rl} - \rho_* a_* \left( x_{*\zeta} \Delta v_{rl} - y_{*\zeta} \Delta u_{rl} \right) \right],
$$

(A.56)

A.14
A.6 Linearizability and Entropy Violation

It is important to note that the recent analysis of Einfeldt et al. [1991] has demonstrated in the case of an ideal gas that not all Riemann problems are linearizable. Their analysis shows that, for some initial data involving strong rarefaction waves or strong shear flows, Roe-type linearized Riemann solvers will produce vacuum states with negative values of density and/or pressure even though the various state pressures and densities of the exact solution are all positive. Refer to the paper by Einfeldt et al. for further details.

It is also now quite well established that finite-difference solution schemes for nonlinear hyperbolic conservation laws, that make use of unmodified Roe-type linearized approximate Riemann solvers, are not in every instance entropy satisfying [Harten, 1983; Roe and Pike, 1984; Sweby and Baines, 1984; Chakravarthy and Osher, 1985a; Chakravarthy, 1987]. Without appropriate entropy corrections or fixes, these schemes permit the formation of stable expansion shocks near sonic points and converge to aphysical solutions. The difficulties near sonic points are discussed in Chapter 4.

A.7 Concluding Remarks

This completes the derivation of the Roe-type approximate Riemann solvers for the conservation equations of inviscid compressible gas dynamics in two-dimensional generalized curvilinear coordinate space. These noniterative solvers may be employed in flux-difference split shock-capturing algorithms for the solution of stationary and nonstationary gaseous flow problems. The Riemann solvers for the case of a thermally and chemically frozen mixture of thermally perfect gases are used in the proposed partially-decoupled TVD schemes of the present numerical study for predicting thermochemical nonequilibrium flows. However, these solvers may also prove to be useful in the computation of compressible flows of polytropic gases with interfaces (i.e., flows with two distinct gases separated by a moving front) [Mulder et al., 1992]. It should be mentioned that Riemann solutions for one- and two-dimensional Cartesian coordinate space can be deduced from the results for the generalized curvilinear coordinate system and extensions of the solvers to the three-dimensional case are possible.
Figure A.1: Wave diagram in the $\zeta$-$t$ plane of self-similar solution to approximate Riemann problem.
Appendix B

Prediction of UTIAS-RPI Hypersonic Impulse Tunnel Performance

B.1 Summary

The hypersonic impulse tunnel of the University of Toronto Institute for Aerospace Studies (UTIAS) and Ryerson Polytechnical Institute (RPI) is a short-duration blow-down experimental wind tunnel capable of producing high Mach number flows ($Ma \approx 8$). A generalized quasi-one-dimensional nonstationary flow analysis and associated total-variation-diminishing finite-difference solution schemes, including approximate Riemann solvers, are presented for predicting the high-temperature flows in such facilities. The analysis is used to investigate the operation of the UTIAS-RPI facility and produce performance data that are not always easily determined or available from experimental measurements. The thermodynamic state of the nozzle-exit flow and high-temperature or real-gas effects are assessed for this facility under various operating conditions. Numerical results, coupled with additional comparisons with available experimental data, demonstrate the range of test-section flows that may be achieved. They also illustrate that for typical operating conditions, the air (working gas used in UTIAS-RPI facility) freezes in the nozzle very close to the throat and results in test-section flows with considerable energy bound in the vibrational modes of the nitrogen ($N_2$) and oxygen ($O_2$) molecules. In particular, the test-section temperatures associated with the vibrational modes of $N_2$ are only marginally less than barrel-end stagnation temperatures, whereas the vibrational temperatures of $O_2$, although lower than stagnation temperatures, are still much higher than the predicted translational-rotational temperatures.

B.2 Introduction

Recently, there has been a renewed interest in hypersonic aerodynamics. The increased research activity in this area was stimulated primarily by a number of major initiatives such as the National Aerospace Plane (NASP) and Aeroassisted Orbital Transfer Vehicle (AOTV) projects in the United States, as well as the European Hermes project. The concept of a viable transatmospheric vehicle for commercial use has also added to this interest.

The physics of hypersonic flow is significantly different from that of the subsonic, transonic, and supersonic flow regimes. Very high temperatures are one characteristic of the hypersonic flow environment. The presence of strong normal shock waves in the stagnation regions of hypersonic flows and the extreme viscous dissipation that occurs within
hypersonic boundary layers can create very high temperatures. For example, atmospheric
re-entry temperatures can reach 11,000 K. Such temperatures are severe enough to excite
vibrational energy modes, cause dissociation, and even ionize the air molecules. For air,
vibrational excitation typically becomes important at temperatures above 800 K, dissociation
of oxygen molecules begins at about 2000 K, and ionization becomes significant once
The occurrence of any or all of these so-called high-temperature or real-gas effects brings
about a dramatic departure in the thermodynamic behaviour of the gas from that of the
ideal. They must be considered in the design of any advanced hypersonic transportation
system, if the problems of surface heating and aerodynamic loading are to be properly
addressed.

Flow scaling or similitude arguments dictate that the vehicle scale must be duplicated, as
well as the velocity and altitude, in any simulation of hypersonic flow undergoing nonequi-
librium chemistry [Hornung, 1988; Lukasiewicz, 1973]. This is not possible in existing
ground-based experimental facilities and full-scale flight tests are required in many cases.
Consequently, computational fluid dynamics (CFD) has become a particularly important
design tool in hypersonic aerodynamics, much more so than for conventional aircraft design.
However, experimental hypersonic research programs are still necessary in order to provide
a reliable experimental data base encompassing a variety of flow conditions for validation of
the CFD computer codes. Furthermore, practical design information can often be obtained
by combining experimental results from several different test facilities.

The so-called impulse, gun, and (or) free-piston shock tunnels [Hornung, 1988; Stalker,
1965; Stalker, 1967; Stalker, 1989; Stollery et al., 1960] are representative of a class of exper-
imental facilities that have been used successfully to simulate various aspects of hypersonic
flight in the laboratory (primarily Mach number and to some extent Reynolds number). A
facility of this sort has been recently refurbished and brought into operation by the Univer-
sity of Toronto Institute for Aerospace Studies (UTIAS) and Ryerson Polytechnical Institute
(RPI) [Deschambault et al., 1989]. In this impulse tunnel, a high pressure driver gas is used
to accelerate a piston. This accelerating piston compresses and heats the working gas (air)
by means of a multiple-shock nonisentropic process for subsequent expansion through a
contoured nozzle to a high Mach number. The use of the piston to separate the driver and
working gases is what differentiates the impulse tunnel from shock tunnels [Hertzberg, 1951;
Hertzberg, 1957; Hornung, 1988; Stalker, 1989; Wittliff et al., 1959], another related class of
hypersonic test facility. Note that impulse tunnels offer several advantages. They generally
have relatively longer run times than alternate intermittent devices such as shock tunnels
and are considerably less costly than continuous or steady-state operating facilities.

The determination of stagnation pressure, stagnation enthalpy or total temperature (a
useful measure of the thermodynamic state of the test-section flow), thermodynamic pro-
cesses in the nozzle of the impulse tunnel, and test-section flow properties are all required
for accurate interpretation of experimental data; however, many of these facility character-
istics are difficult to measure directly. Furthermore, a thorough understanding of the tunnel
operation is required in order to explore various avenues for extending the range of flow
conditions that may be simulated. Previous studies have generally employed simplified an-
alytic techniques to investigate various aspects of tunnel performance (see, for example, the
work of Evans and Evans [1956], Lemcke [1962], Stalker [1961], Stollery and Maull [1958],
Stollery and Smith [1962], Stollery and Park [1963], and Winter [1960]). More recently, a
simplified quasi-one-dimensional numerical model has been proposed for the starting pro-
cess in the nozzle of a free-piston shock tunnel [Jacobs, 1991]. This appendix presents a
fairly sophisticated quasi-one-dimensional nonstationary compressible flow analysis and related numerical solution algorithm that have been developed for predicting the complete unsteady performance and operation of the UTIAS-RPI hypersonic impulse tunnel. The analysis is capable of predicting barrel stagnation and test-section flow properties, unsteady piston motion, run times, as well as the high-temperature effects associated with the impulse tunnel flows. Modeling and algorithm details, comparisons with experimental data, and predictions of tunnel performance are all described. The analysis and results presented here are also described by Groth et al. [1991].

B.3 Description of Impulse Tunnel

The UTIAS-RPI hypersonic impulse tunnel is a blow-down or short-duration test facility in which the high stagnation temperatures for the nozzle flows are generated by a shock compression process. A schematic of the experimental facility is depicted in Figure B.1a. The tunnel consists of a 5.6 m long reservoir or driver with an internal radius of 152.4 mm and a 6.4 m long barrel with an internal radius of 38.1 mm that are separated by an isolating ball valve and a double diaphragm. A relatively light aluminum piston weighing approximately 95 g is free to move in the barrel. Various convergent-divergent nozzles may be connected to the barrel at the nozzle breech. A 1.54 m long nozzle with throat and exit radii of 6.35 and 108.87 mm, respectively, is currently employed. This nozzle has a design Mach number of 8.33. The nozzle projects into a 0.61 m long test section with a rectangular cross section of 0.61 \times 0.64 \text{ m}^2, which is in turn connected by a diffuser to a relatively large dump tank with a volume of approximately 2.85 \text{ m}^3. The initial pressure of the driver gas (currently air) in the reservoir is normally maintained at 20.5 MPa and initial barrel pressure for the working gas (again this is usually air) ranges between 200 and 800 kPa. A small Lexan plug is placed in the throat of the nozzle so that the test section can be evacuated down to pressures nearing 50 Pa.

During tunnel operation, the double diaphragm is burst and the high-pressure driver gas rapidly accelerates the piston along the barrel. The accelerating piston creates a series of multiple shock reflections in the barrel that heat and compress the working gas. The nozzle throat plug is expelled by the first reflected shock and the working gas then flows through the convergent-divergent nozzle and on through the test section. The piston eventually comes to rest at the end of the barrel when the working gas is depleted. Typical run times for this facility are between 10–30 ms. The impulse tunnel operation is illustrated in the x-t wave diagram of Figure B.1b. The primary shock and rarefaction wave patterns characterizing the nonstationary wave interaction processes occurring in the tunnel, indicated by $\tilde{S}$ and $\tilde{R}$ respectively, are shown in this figure. Note that a more complete description of the UTIAS-RPI hypersonic impulse tunnel, which includes details of tunnel instrumentation and calibration, is given by Deschambault et al. [1989].

B.4 Equations of Motion

The complex unsteady flow of the driver and working gases in the reservoir, barrel, and nozzle behind and in front of the accelerating piston are modeled by solving the equations of motion (continuity, momentum, and energy) for generalized one-dimensional nonstationary compressible flows in ducts. The equations include inhomogeneous source terms associated with the flow driving potentials of area change, friction, heat transfer, and head loss and
are well documented in many textbooks (see, for example, the text by Zucrow and Hoffman [1976]). They have been used successfully in previous studies to predict nonstationary flows in other experimental facilities such as blast-wave simulators and two-stage light-gas hypervelocity launchers [Gottlieb et al., 1989; Groth and Gottlieb, 1988; Zhang and Gottlieb, 1986]. The weakly conservative forms of these partial differential equations may be expressed as

$$\frac{\partial}{\partial t} (U) + \frac{\partial}{\partial x} [F(U)] = A(U) + S(U), \quad (B.1)$$

where the multi-component solution and flux column vectors $U$ and $F$ are given by

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho (e + \frac{1}{2} u^2) \end{bmatrix} \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u \left( e + \frac{p}{\rho} + \frac{1}{2} u^2 \right) \end{bmatrix}, \quad (B.2)$$

the source column vectors $A$ and $S$ are defined by

$$A = \begin{bmatrix} -\rho u \frac{1}{A} \frac{dA}{dx} \\ -\rho u^2 \frac{1}{A} \frac{dA}{dx} \\ -\rho u \left( e + \frac{p}{\rho} + \frac{1}{2} u^2 \right) \frac{1}{A} \frac{dA}{dx} \end{bmatrix} \quad S = \begin{bmatrix} 0 \\ F_{wall} + F_{loss} \\ Q_{wall} + Q_{zero} \end{bmatrix}, \quad (B.3)$$

and the symbols $\rho$, $u$, $p$, and $e$ denote the gas density, velocity, pressure, and total specific internal energy, and $x$ and $t$ are position and time. The variable $A$ is the local cross-sectional area of the duct which is taken to be a known function of $x$. The other terms appearing in column vectors $A$ and $S$ represent the effects of area change, boundary-layer friction, wall heat transfer, and other flow pressure or head losses. $F_{wall}$ is an equivalent body force per unit volume to account for viscous or frictional losses in the boundary layer near the wall of the duct flow. $F_{loss}$ is a similar body force per unit volume that includes additional pressure losses for flows through area changes and over diaphragm remnants. The variable $Q_{wall}$ denotes the heat transfer rate per unit volume from the duct walls to the gas and the variable $Q_{zero}$ represents the time rate of change in the zero-point energy of the gas resulting from chemical reactions. This latter term is required when modeling finite-rate reaction processes.

The body force due to boundary layer friction can be expressed in the form

$$F_{wall} = -\frac{f}{D_h} \frac{\rho u |u|}{2}, \quad (B.4)$$

where $f$ is the Darcy-Weisbach friction factor and $D_h$ is the local hydraulic diameter of the duct ($D_h = 2\pi r$ for pipes where $r$ is the radius). The friction factor is evaluated using
for which \( \text{Re} = \rho |u| D_h / \mu \) is the local Reynolds number, \( \mu \) is the gas viscosity, and \( \varepsilon \) denotes the absolute roughness of the wall surface. The previous relationships are taken from steady pipe flow theory. The first expression is the well-known theoretical result from Hagen-Poiseuille flow which describes the friction factor in the laminar regime (\( 0 < \text{Re} < 2000 \)), the third is an explicit empirical expression developed by Jain [1976] valid in the fully turbulent regime (\( \text{Re} > 4000 \)), and the other expression provides estimates for the friction factor in the transitional regime (\( 2000 \sim \text{Re} \sim 4000 \)). Note that \( \Lambda \) is a compressibility correction factor. It is calculated from the semi-empirical relation \( \Lambda = 1 + (\gamma - 1)\Omega Ma^2/2 \) as suggested by Liepmann and Goddard [1957], where \( \gamma \) is the specific heat ratio of the gas, \( Ma \) is the local flow Mach number, and \( \Omega \) is the recovery factor. This last parameter can be approximated by \( Pr^{1/2} \) for laminar flows and \( Pr^{1/3} \) for turbulent flows where \( Pr \) is the Prandtl number for the gas.

Similarly, the body forces due to pressure or head losses in the flow can be written as

\[
F_{\text{loss}} = -\frac{K \rho u|u|}{L},
\]

where \( K \) is the head-loss coefficient and \( L \) is the finite duct length over which the losses are distributed (\( L = 2D_h \) in this study). Although these losses are usually small, values for \( K \) can range between 0–10 depending on the flow obstructions.

The rate of heat transfer to the gas from the wall per unit volume of the flow \( Q_{\text{wall}} \) is prescribed by employing the semi-empirical form of Reynolds’ analogy for compressible pipe flow suggested by Colburn [Kreith, 1967]. The heat transfer rate is thus given by

\[
Q_{\text{wall}} = 4k \frac{Nu}{D_h^2} [T_w - T_{aw}] = \frac{f C_p \rho |u|}{2 Pr^{2/3} D_h} [T_w - \Lambda T],
\]

where \( Nu, k, \) and \( C_p, T, \) and \( T_{aw} \) are the gas Nusselt number, thermal conductivity, specific heat at constant pressure, temperature, and adiabatic wall temperature, respectively, and \( T_w \) is the local duct wall temperature. Note that the Prandtl number is defined by \( Pr = \mu C_p / k \) and the effects of compressibility appear in Eq. (B.7) via the friction factor \( f \) and correction factor \( \Lambda \).

The piston of the UTIAS-RPI hypersonic impulse tunnel is basically a thick aluminum disc with a trailing tapered skirt that provides stability during motion. Holes are machined through the skirt to reduce weight. In order to model the piston motion in the barrel, it is assumed that the piston is a rigid cylinder of length \( L_p \) and radius \( r_p \). Newton’s law is then applied with pressure, inertial, and viscous drag forces all taken into account. This results in a differential equation for the piston motion which can be written as

\[
m_p \frac{dV_p}{dt} = \pi r_p^2 (p_f - p_b) + F_p,
\]
where $V_p$ is the piston velocity, $p_f$ and $p_b$ are the front and back face pressures exerted on the piston by the high-pressure gases, $F_p$ is the frictional force acting on the piston, and $m_p$ is the piston mass. The friction force is determined by assuming that a quasi-steady Couette flow exists between the exterior surface of the piston and the tunnel walls and a Reynolds number correlation similar to those for fully developed pipe flow is used to determine the frictional shear stress at the piston surface. $F_p$ can then be approximated by

$$F_p = -2\pi r_p L_p (1 - \sigma) f_p \left[ \frac{\mu V_p}{r - r_p} \right] \text{,} \quad (B.9)$$

where $f_p$ is the piston friction factor having the form $f_p = c R e_p^n$ and $R e_p = \rho |V_p|(r - r_p)/\mu$ is the piston Reynolds number; $c$ and $n$ are constants. The variable $\sigma$ ($0 \leq \sigma < 1$) is the porosity of the piston skirt.

### B.5 Thermodynamic Models for Air

At the present time, air is used almost exclusively as the driver and working gas in the UTIAS-RPI hypersonic impulse tunnel. Thermodynamic and caloric models are required to interrelate the various intensive properties of air, such as pressure, temperature, and internal energy, and thereby complete or close the governing set of equations given by Eqs. (B.1)–(B.7). In this study, three different models are employed to describe the thermodynamic and transport properties of air. They are the perfect-gas model (polytropic or thermally and calorically perfect gas), an equilibrium real-gas model, and a nonequilibrium (vibrationally relaxing and chemically reacting) high-temperature model. The three different thermodynamic models are very helpful in assessing the magnitude of the high-temperature effects in the impulse tunnel flows and the departure of the working gas behaviour from the ideal.

#### B.5.1 Polytropic Model

For polytropic gases, the pressure and temperature can be related to the density and total specific internal energy using the well-known ideal-gas equation of state

$$p = \rho RT = (\gamma - 1)\rho e \text{,} \quad (B.10)$$

where $\gamma$ is the specific heat ratio, $R$ is the gas constant, and $C_p = \gamma R / (\gamma - 1)$. In the case of air, the values of $\gamma$ and $R$ are taken to be 1.40 and 287.06 Pa·m$^3$/kg·K, respectively. The sound speed $a$ can also be related to the other intensive properties by the expressions

$$a^2 = \gamma RT = \frac{\gamma p}{\rho} = \gamma(\gamma - 1)e \text{.} \quad (B.11)$$

The polytropic model is completed by employing semi-empirical expressions for the dynamic viscosity and Prandtl number. An empirical extension of Sutherland's law of the form

$$\mu = \frac{c_1 T^{3/2}}{c_2 + T^{c_3} + c_4 / T} \text{,} \quad (B.12)$$

is used, where $c_1$, $c_2$, $c_3$, and $c_4$ are constants and equal to $5.2192 \times 10^{-7}$, $-3.31132$, $0.865351$, and $5.2192 \times 10^{-7}$, respectively.
and 2365.27, respectively, for air. The Prandtl number for air depends primarily on the specific heat ratio. A modified form of Euken's formula is used herein to prescribe the Prandtl number. The formula is based on some ideas of Chapman and Cowling [1970] and given by

\[ Pr = \frac{20\gamma}{39\gamma - 15}, \]  

(B.13)

which is in good agreement with experimental data.

### B.5.2 Equilibrium Model

The curve fits of Srinivasan et al. [1987] and Srinivasan and Tannehill [1987] are used to represent the equilibrium thermodynamic and transport properties of air. These curve fits are constructed from bicubic polynomials and Grabau-type transition functions to model the thermodynamic properties in a piecewise manner. They are valid for temperatures up to 25,000 K. The correlations for the pressure \( p \), temperature \( T \), sound speed \( a \), viscosity \( \mu \), Prandtl number \( Pr \), and thermal conductivity \( k = \mu C_p / Pr \) in the form \( p = p(\rho, e) \), \( T = T(\rho, e) \), \( a = a(\rho, e) \), \( \mu = \mu(\rho, T) \), \( Pr = Pr(\rho, T) \), and \( k = k(\rho, e) \) are all employed. Note that if the equation of state has the form \( p = p(\rho, e) \), then the sound speed can be related to the pressure, density, and internal energy by the relationship

\[ a^2 = \frac{\partial p}{\partial \rho} = \frac{\partial p}{\partial \rho} + \frac{p}{\rho^2} \frac{\partial p}{\partial e}, \]  

(B.14)

where \( s \) is the entropy.

### B.5.3 Nonequilibrium Model

The thermodynamics of the nonequilibrium air is modeled by treating it as a chemically reactive mixture of thermally perfect gases for which the thermal state can be described by the following separate and independent temperatures (or internal energies): a translational-rotational temperature and the vibrational temperatures of the polyatomic species. The translational-rotational temperature represents the contribution to the internal energy by the translational and rotational modes of all molecules and atoms in the mixture. These modes are assumed to be in equilibrium, which is a reasonable approximation for most continuum flow studies [Vincenti and Kruger, 1975]. Each vibrational temperature represents the contribution to the internal energy by the vibrational modes of the corresponding polyatomic species. Intermolecular forces, electronic excitation, and ionization effects are all neglected.

Additional equations for species mass and vibrational energy are necessary for describing the one-dimensional flow of a nonequilibrium mixture. They may be written as [Gnoffo et al., 1989]

\[ \frac{\partial W}{\partial t} + u \frac{\partial W}{\partial x} = Q(W), \]  

(B.15)

where the column vectors \( W \) and \( Q \) are defined by

B.7
and where \( c_s = \rho_s / \rho \) is the mass fraction of species \( s \) with \( \sum_s c_s = 1 \), \( \rho_s \) is the density of species \( s \), \( e_{vs} \) is the specific vibrational energy of species \( s \), \( e_v = \sum_s c_s e_{vs} \) is the total specific vibrational energy of the mixture, and \( N \) is the number of species in the mixture. The variable \( w_s \) represents the time rate of change of the concentration of the species \( s \) brought about by the chemical reactions. The variable \( q_s \) represents the time rate of change of the vibrational energy of the species \( s \) brought about by relaxation to its equilibrium value. Finally, the term \( \beta_s w_s e_{vs} \) appearing in Eqs. (B.15) and (B.16) is related to the change in the vibrational energy of species \( s \) per unit volume of the mixture due to the chemical reactions. The quantity \( \beta_s \) is an empirical value greater than or equal to unity. It is introduced to reflect the observed preference of higher-than-average vibrationally excited molecules to dissociate and the tendency of atoms to combine and form higher-than-average vibrationally excited molecules [Gnoffo et al., 1989].

The total specific internal energy of the thermally perfect gaseous mixture is the sum of translational-rotational and vibrational energies and given by

\[
e = e_{tr} + e_v = e_{tr} + \sum_{s=1}^{N} c_s e_{vs},
\]

where \( e_{tr} \) is the translational-rotational energy. The mixture pressure may then be expressed in terms of the translational-rotational temperature \( T \) and (or) energy \( e_{tr} \) and the various mixture properties by employing the ideal equation of state for each thermally perfect species and applying Dalton’s law of partial pressure. The resulting equation of state for the mixture is

\[
p = \rho RT = (\gamma - 1)\rho e_{tr},
\]

where \( R = \mathcal{R}(\sum_s c_s/M_s) = \sum_s c_s R_s \) is the specific gas constant of the mixture, \( \mathcal{R} \) is the universal gas constant, \( M_s \) is the molecular weight of species \( s \), \( R_s = \mathcal{R}/M_s \) is the specific gas constant of species \( s \), and \( \gamma = 1 + [\sum_s c_s R_s]/[\sum_s c_s R_s/(\gamma_s - 1)] \) is defined to be the frozen specific heat ratio of the mixture. The variable \( \gamma_s \) represents the frozen specific heat ratio of species \( s \) (i.e., the specific heat ratio of the species in the absence of vibrational excitation). It is also possible to define a frozen sound speed for the mixture. This intensive property may be related to the other mixture properties by the expression

\[
a^2 = \gamma RT = \gamma \frac{p}{\rho} = \gamma(\gamma - 1)e_{tr},
\]

where \( a \) is the frozen sound speed.

In this work, a five-species (\( \text{N}_2, \text{O}_2, \text{NO}, \text{N}, \) and \( \text{O} \)) four-temperature (i.e., translational-
rotational temperature $T$, and vibrational temperatures $T_{vN_2}$, $T_{vO_2}$, and $T_{vNO}$) nonequilibrium thermodynamic model of air is employed. This model, which is described below, is valid for temperatures up to 8000 K and pressures above 0.10 kPa. Note that additional and in some instances more complete information concerning the model is given in Appendix C.

In the five-species four-temperature model, the chemical reaction mechanism of air is represented by the elementary reactions

\[
\begin{align*}
N_2 + M &= 2N + M, \\
O_2 + M &= 2O + M, \\
NO + M &= N + O + M, \\
NO + O &= N + O_2, \\
N_2 + O &= NO + N,
\end{align*}
\]

(B.20)

where $M$ is a collision partner; it can be any one of the five species. Seventeen elementary reactions (fifteen dissociation/recombination and two exchange reactions) are represented by the reaction scheme of Eq. (B.20). Collision theory is used to describe these finite-rate reaction processes from which empirical expressions for the time rate of change of the species concentrations may be obtained. These expressions have the form [Anderson, 1982; Anderson, 1989; Vincenti and Kruger, 1975]

\[
w_s = \frac{M_s}{\rho} \sum_{r=1}^{N_R} \left( \sigma_{s,r}^b - \sigma_{s,r}^f \right) \left\{ k_f^r \prod_{s'=1}^{N} \left( \frac{c_{s',r} \rho}{M_{s'}} \right) \sigma_{s',r}^f - k_r^b \prod_{s'=1}^{N} \left( \frac{c_{s',r} \rho}{M_{s'}} \right) \sigma_{s',r}^b \right\},
\]

(B.21)

where $\sigma_{s,r}^f$ and $\sigma_{s,r}^b$ are the stoichiometric coefficients of the reactant and product species $s$ for the reaction $r$, and $k_f^r$ and $k_r^b$ are the forward and backward reaction rates of reaction $r$. The variable $N_R$ represents the total number of elementary reactions. The reaction rates are assumed to be functions of the rotational-translational temperature and are described by modified forms of the Arrhenius equation. They are given by

\[
k_f^r = C_r^f T_r^{n_f^r} \exp \left( \frac{-E_r^f}{KT} \right), \quad k_r^b = C_r^b T_r^{n_r^b} \exp \left( \frac{-E_r^b}{KT} \right).
\]

(B.22)

The reaction rate coefficients $C_r^f$, $C_r^b$, $n_f^r$, $n_r^b$, $E_r^f$, and $E_r^b$ of Eq. (B.22) are taken from the data set compiled by Dunn and Kang [1973].

The finite-rate vibrational relaxation of the diatomic molecules is represented in the five-species four-temperature nonequilibrium model of air by assuming that the vibrationally excited molecules behave as ideal harmonic oscillators. It is further assumed that the relaxation process from an excited nonequilibrium state to a state of thermodynamic equilibrium (i.e., $T = T_{vN_2} = T_{vO_2} = T_{vNO}$) occurs only through translational-vibrational collisions. Under these assumptions, it is possible to prescribe the time rate of change of the vibrational energy of the species $s$ by [Anderson, 1982; Anderson, 1989; Vincenti and Kruger, 1975]

\[
q_s = \frac{e_{v_s}^* - e_{v_s}}{\tau_s},
\]

(B.23)

where $e_{v_s}^*$ is the equilibrium vibrational energy given by

\[
e_{v_s}^* = \frac{\Theta_{v_s} R_s}{\exp(\Theta_{v_s}/T) - 1},
\]

(B.24)
and \( \tau_s \) is the characteristic relaxation time. The characteristic vibrational temperatures \( \Theta_{vN_2}, \Theta_{vO_2}, \) and \( \Theta_{vNO} \) are taken to be 3353, 2239, and 2699 K, respectively. The semi-empirical correlations of Millikan and White [1963] based on modifications to the Landau-Teller equation are used to determine \( \tau_s \). These correlations have the form

\[
\tau_s = \frac{\sum_{s'} c_{s'} \exp[A_s(T^{-1/3} - 0.015(\frac{M_s M_{s'}}{M_s + M_{s'}})^{1/4}) - 18.42]}{\rho \sum_{s'} c_{s'}} ,
\]

and \( A_{N_2}, A_{O_2}, \) and \( A_{NO} \) are assumed to have values of 220, 129, and 168, respectively.

Using the preceding relations, it is possible to prescribe the source term \( Q_{zero} \) of Eq. (B.1) that represents the total change in the zero-point energy of the mixture resulting from the chemical reactions by the expression

\[
Q_{zero} = -\rho \sum_{s=1}^{N} w_s \Delta h^0_{f_s} ,
\]

where \( \Delta h^0_{f_s} \) is the heat of formation of species \( s \) evaluated at a temperature of 0 K. The heats of formation for the five species were taken to be \( \Delta h^0_{fN_2} = 0, \Delta h^0_{fO_2} = 0, \Delta h^0_{fNO} = 2991.89 \) kJ/kg, \( \Delta h^0_{fN} = 33613.91 \) kJ/kg, and \( \Delta h^0_{fO} = 15424.95 \) kJ/kg. Note that \( Q_{zero} \) is identically zero for the polytropic and equilibrium models. Note additionally that the effect of the preferential dissociation of vibrationally excited diatomic molecules is not included herein and \( \beta_s \) is taken to be unity in this work.

Finally, transport properties of nonequilibrium air required for the determination of the boundary-layer friction \( F_{wall} \) and heat transfer \( Q_{wall} \) in Eqs. (B.1)-(B.3) are computed as follows. The mixture specific heat and Prandtl number are approximated by the frozen flow (i.e., polytropic-gas equivalent) relations \( C_p = \gamma R/\gamma - 1 \) and \( Pr = 20\gamma/(39\gamma - 15) \), respectively. The viscosity of each species \( \mu_s \) is defined in terms of the translational-rotational temperature \( T \) by using the semi-empirical correlations of Blottner et al. [1971] given by

\[
\mu_s = 0.10 \exp[(b_1 + b_2) + b_3 + b_3] ,
\]

and the mixture or total viscosity is calculated by employing the semi-empirical mixing rule of Wilke [1950] as follows:

\[
\mu = \sum_{s=1}^{N} \frac{c_s \mu_s}{M_s \phi_s} ,
\]

where

\[
\phi_s = \sum_{s' = 1}^{N} \frac{c_{s'} M_{s'}}{M_s} \left[ 1 + \left( \frac{\mu_s}{\mu_{s'}} \right)^{1/2} \left( \frac{M_{s'}}{M_s} \right)^{1/4} \right]^2 \left[ 8 \left( 1 + \frac{M_{s'}}{M_s} \right) \right]^{-1/2} .
\]

The curve fits of Eq. (B.27) are appropriate for temperatures up to 10,000 K. Values for the constant coefficients \( b_1, b_2, \) and \( b_3 \), for each species are taken from the work of Blottner et al. [1971].
B.6 Numerical Solution Procedure

General solutions to the preceding equations prescribing the flow of the impulse tunnel driver and working gases and the motion of the piston in the barrel and must be obtained numerically. The differential equation for the piston motion given by Eq. (B.8) can be integrated by decoupling it from the gas dynamic equations and employing the most recent flow field solution in a forward Euler time-stepping procedure. This simple approach is sufficiently accurate and robust as the characteristic time scales associated with the piston motion are very much larger than the gas dynamic time scales. The gas dynamic equations given by Eqs. (B.1)–(B.3) may then be solved in a separate integration procedure where, at each level or time step, the corresponding updated solution for the piston motion is employed. However, the numerical solution of this inhomogeneous system of hyperbolic conservation laws is made difficult by the presence of large solution gradients and strong shocks. It is further complicated if source terms are stiff. Classical first-order shock-capturing finite-difference schemes can require excessive grid refinement to resolve the complicated shock structure, and second-order schemes can lead to spurious Gibb’s-like oscillations or nonlinear instabilities near discontinuities. In the last 5–10 years, solution-dependent nonlinear higher-order methods have been developed, such as the total-variation-diminishing (TVD) finite-difference schemes of Harten [1983; 1984], Roe [Roe, 1981; Roe and Pike, 1984; Roe, 1984], Davis [1984], Yee [1987a], and Chakravarthy and Osher [1985a; 1985b]. They are very appropriate for the hyperbolic system considered here. These schemes effectively eliminate oscillations near extrema, limit numerical diffusion, maintain higher-order accuracy wherever possible, and thereby permit the efficient resolution of weak solutions.

In this study, the explicit higher-order TVD upwind difference scheme of Roe [Roe, 1981; Roe and Pike, 1984; Sweby, 1984] is used to solve the governing partial differential equations of the gaseous flows when supplemented by the ancillary equations of the polytropic and equilibrium thermodynamic models. Roe’s approximate Riemann solver is used in the evaluation of the numerical fluxes for the polytropic case and an extension of this approximate solver proposed by Glaister [1988a] is employed for the equilibrium case.

When supplemented with nonequilibrium thermodynamic model equations, the solution of Eq. (B.1) is complicated by the additional species mass and vibrational energy conservation equations Eq. (B.15), as well as the presence of inhomogeneous source terms representing the finite-rate vibrational relaxation and chemical reaction processes. The additional source terms are often large and can make the solution algorithms stiff (i.e., the time stepping of a marching procedure is drastically constrained by stability considerations rather than by the usual accuracy concerns). In this case, the gas dynamic and thermodynamic equation sets are partially decoupled by employing a frozen flow approximation. Both sets of decoupled equations are then integrated alternately in a lagged manner within a time marching procedure. A semi-implicit version of the Roe’s scheme is applied to each equation set. The inhomogeneous source terms associated with the finite-rate processes are treated implicitly in the time-stepping scheme and an extension of Roe’s approximate Riemann solver is used to evaluate the numerical flux functions. The extended Riemann solver provides the eigenvalues and eigenvectors of the fully coupled system.

Further details of these TVD shock-capturing schemes are given in the following sub-sections. The various algorithm extensions particular to the present application are discussed. This includes the approximate Riemann solvers, partial-decoupling procedure, implicit treatment of stiff source terms, and boundary conditions.
B.6.1 Solution Algorithm for Polytropic and Equilibrium Gas Flows

TVD schemes were originally developed for solving linear and nonlinear scalar homogeneous hyperbolic conservation laws in one space dimension. Algorithm extensions are necessary to deal with the vector nature and source terms of inhomogeneous systems of differential equations. In Roe's flux-differencing method, a local characteristic approach is adopted in which the properties of the inviscid flux Jacobians are utilized in conjunction with approximate Riemann solvers to represent the solution and flux vector jumps in terms of characteristic variables. A TVD algorithm is then applied to each characteristic field in a scalar fashion. Source terms may be treated either explicitly or implicitly depending on the nature of the equations.

In the case of the polytropic and equilibrium thermodynamic models, Roe method solutions of the one-dimensional three-component system given by Eq. (B.1) can be formulated as follows. Let $U^n_i$ be the numerical approximation of the solution at discrete locations $x = x_i$ and time $t = t^n$. The solution at subsequent time levels is obtained by means of the time-stepping procedure

$$U^{n+1}_i = L_{U}^{i+1/2} U^n_i,$$

where the solution operator $L_{U}^{i+1/2}$ advances the solution $U$ through a time interval $\Delta t^n$ with $\Delta t^n = t^{n+1} - t^n$ and is defined by the two-stage difference scheme

$$U^{n+1}_i = U^n_i + \Delta U^n_i = U^n_i + \Delta t^n (A^n_i + S^n_i) -$$

$$\frac{1}{2} \sum_{k=1}^{3} \left\{ \left[ (\nu_{i+1/2,k} - |\nu_{i+1/2,k}|) + \phi_{i+1/2,k} |\nu_{i+1/2,k}| (1 - |\nu_{i+1/2,k}|) \right] \Delta U^n_{i+1/2,k} +

\left[ (\nu_{i-1/2,k} - |\nu_{i-1/2,k}|) - \phi_{i-1/2,k} |\nu_{i-1/2,k}| (1 - |\nu_{i-1/2,k}|) \right] \Delta U^n_{i-1/2,k} \right\}, \quad \text{(B.31)}$$

$$U^{n+1}_i = U^n_i + \Delta U^n_i = U^{n+1/2}_i + \frac{1}{2} \Delta t^n \left( A^{n+1}_i - A^n_i + S^{n+1}_i - S^n_i \right), \quad \text{(B.32)}$$

and where $\Delta U^n_i = U^{n+1}_i - U^n_i$, $\Delta U^{n+1}_i = U^{n+1}_i - U^n_i$, and $U^{n+1/2}_i$ denotes an intermediate solution state. The quantities $\nu_{i+1/2,k}^n$ and $\Delta U^n_{i+1/2,k}$ appearing in Eq. (B.31) are the local average Courant-Friedrichs-Lewy (CFL) number and solution jump vector associated with the $k$th elemental wave of the $i$th approximate Riemann problem posed between the $i$th and $i+1$ nodes of the spatial grid. They may be related to the eigenvalues and eigenvectors of the Jacobian of the homogeneous flux vector $J = \partial F/\partial U$ by employing Roe's approximate Riemann solver. The CFL numbers and solution jump vectors can be defined by

$$\nu_{i+1/2,k}^n = \frac{\Delta t^n \lambda_{i+1/2,k}^n}{\Delta x_{i+1/2}}, \quad \text{(B.33)}$$

$$\Delta U^n_{i+1/2,k} = \alpha_{i+1/2,k}^n e_{i+1/2,k}^n, \quad \text{(B.34)}$$

with $\Delta x_{i+1/2} = x_{i+1} - x_i$, and where $\lambda_{i+1/2,k}^n$ and $e_{i+1/2,k}^n$ are the $k$th eigenvalue and...
eigenvector of the flux Jacobian evaluated at an appropriate average state $U_{i+1/2}^n$. The variable $\alpha_{i+1/2,k}^n$ is the strength of the $k$th elemental wave. The eigenvalues of the Jacobian $J = \partial F/\partial U$ are given by

$$
\lambda_{i+1/2,1}^n = u_{i+1/2}^n - a_{i+1/2}^n, \quad \lambda_{i+1/2,2}^n = u_{i+1/2}^n, \quad \lambda_{i+1/2,3}^n = u_{i+1/2}^n + a_{i+1/2}^n,
$$

and the eigenvectors can be written as

$$
e_{i+1/2,1}^n = \begin{bmatrix} 1 \\ u_{i+1/2}^n - a_{i+1/2}^n \\ h_{i+1/2}^n - u_{i+1/2}^n a_{i+1/2}^n \end{bmatrix}, \quad e_{i+1/2,2}^n = \begin{bmatrix} 1 \\ u_{i+1/2}^n + a_{i+1/2}^n \\ h_{i+1/2}^n + u_{i+1/2}^n a_{i+1/2}^n \end{bmatrix}, \quad e_{i+1/2,3}^n = \begin{bmatrix} 1 \\ a_{i+1/2}^n \\ 1 - \frac{\partial \rho}{\partial e} \bigg|_{i+1/2} \end{bmatrix},
$$

where $a_{i+1/2}^n$ is the local average state sound speed and $h = e + p/\rho + u^2/2$ is the specific enthalpy. Note that for polytropic gases, $\partial p/\partial e = (\gamma - 1)\rho$ and, therefore, $h - p\alpha^2/(\partial p/\partial e) = u^2/2$. Using the condition $\Delta U_{i+1/2}^n = U_{i+1}^n - U_i^n = \sum_k \alpha_{i+1/2,k}^n e_{i+1/2,k}^n$, it is possible to relate the elemental wave strengths to the average state values of the primitive variables $\rho_{i+1/2}^n, u_{i+1/2}^n, e_{i+1/2}^n, p_{i+1/2}^n, a_{i+1/2}^n$, and $h_{i+1/2}^n$, and the solution jumps $\Delta \rho_{i+1/2}^n = \rho_{i+1}^n - \rho_{i}^n$, $\Delta u_{i+1/2}^n = u_{i+1}^n - u_{i}^n$, and $\Delta p_{i+1/2}^n = p_{i+1}^n - p_{i}^n$. The resulting expressions are

$$
\alpha_{i+1/2,1}^n = \frac{1}{2(a_{i+1/2}^n)^2} \left[ \Delta \rho_{i+1/2}^n - \rho_{i+1/2}^n a_{i+1/2}^n \Delta u_{i+1/2}^n \right],
$$

$$
\alpha_{i+1/2,2}^n = \Delta \rho_{i+1/2}^n - \frac{\Delta p_{i+1/2}^n}{(a_{i+1/2}^n)^2},
$$

$$
\alpha_{i+1/2,3}^n = \frac{1}{2(a_{i+1/2}^n)^2} \left[ \Delta \rho_{i+1/2}^n + \rho_{i+1/2}^n a_{i+1/2}^n \Delta u_{i+1/2}^n \right].
$$

In deriving these wave strengths, it has been assumed that linearized approximations such as $\Delta (\rho u)^n_{i+1/2} = \rho_{i+1/2}^n \Delta u_{i+1/2}^n + u_{i+1/2}^n \Delta \rho_{i+1/2}^n$ apply in the more general case where the solution jumps are large.

For polytropic gases obeying the ideal equation of state, Roe [1981] has constructed approximate Riemann problem solutions and shown that the appropriate average state $U_{i+1/2}^n$ should be defined as follows:

$$
\rho_{i+1/2}^n = \sqrt{\rho_{i+1}^n \rho_{i}^n}.
$$

B.13
These averages guarantee conservation and afford the difference scheme excellent shock-capturing attributes (using the preceding definition of the average state, the approximate Riemann solution is exact for the case of a single discontinuity). Glaister [1988a] has since extended Roe’s approximate solution to the more general case of equilibrium real-gas equations of state that have the form $p = p(\rho, e)$. In this case, the preceding averages for $\rho$, $u$, $e$, $h$, and $p$ given by Eqs. (B.41)-(B.44) are still applicable, but additional relations are required for determining local average-state values for the partial derivatives of the pressure with respect to the density and internal energy and for evaluating an average-state sound speed. Glaister’s proposed averages for $\partial p/\partial \rho$ and $\partial p/\partial e$ are

$$\frac{\partial p}{\partial \rho}_{i+1/2} = \left\{ \begin{array}{ll}
\frac{1}{2\Delta \rho} \left[ (p(\rho^n_{i+1}, e^n_{i+1}) + p(\rho^n_{i+1}, e^n_{i+1})) - [p(\rho^n_{i+1}, e^n_{i+1}) + p(\rho^n_{i+1}, e^n_{i+1})] \right] \\
\frac{1}{2} \left[ \frac{\partial p}{\partial \rho}_{i+1} + \frac{\partial p}{\partial \rho}_{i} \right] \end{array} \right\}, \quad \Delta \rho^n_{i+1/2} \neq 0, \quad \Delta \rho^n_{i+1/2} = 0,$$

$$\frac{\partial p}{\partial e}_{i+1/2} = \left\{ \begin{array}{ll}
\frac{1}{2\Delta e} \left[ (p(\rho^n_{i+1}, e^n_{i+1}) + p(\rho^n_{i+1}, e^n_{i+1})) - [p(\rho^n_{i+1}, e^n_{i+1}) + p(\rho^n_{i+1}, e^n_{i+1})] \right] \\
\frac{1}{2} \left[ \frac{\partial p}{\partial e}_{i+1} + \frac{\partial p}{\partial e}_{i} \right] \end{array} \right\}, \quad \Delta e^n_{i+1/2} \neq 0, \quad \Delta e^n_{i+1/2} = 0,$$

and $a$ is then specified using Eq. (B.14) by the expression

$$a^n_{i+1/2} = \left[ \frac{\partial p}{\partial \rho}_{i+1/2} + \frac{p^n_{i+1/2}}{(\rho^n_{i+1/2})^2} \right]_{i+1/2}^{1/2}. \quad (B.47)$$

Although other averages for the derivatives of the pressure have been proposed, see for example Liou et al. [1990], this choice of averaging has been demonstrated to provide accurate solutions in a relatively efficient manner.

The higher-order flux-differencing scheme of Roe is a smart solution adaptive method that provides improved numerical accuracy and monotonic or oscillation-free solutions by having difference coefficients that depend on the local solution at each time step. The underlying constant-coefficient or unlimited scheme is a combination of the second-order schemes of Lax and Wendroff [1960] (central differences) and Warming and Beam [1976] (upwind differences). Flux limiters are employed to limit the magnitude of the second-order antidiffusive fluxes and reduce the scheme to the first-order fully-upwind method of Cole and Murman [Murman, 1974] at local extrema of the solution. In the case of
linear and nonlinear scalar homogeneous hyperbolic conservation laws and linear systems of homogeneous conservation laws, the resulting nonlinear scheme is TVD [Harten, 1983; Harten, 1984], which guarantees that the scheme is monotonicity preserving. In the more general case of nonlinear inhomogeneous systems as given by Eq. (B.1), numerical experiments provide evidence that Roe’s flux-limited scheme has good shock-capturing capabilities. The term ‘higher-order’ is applied to Roe’s method to indicate that the formal accuracy of the scheme with uniform computational domain is second order for regions where the solution is smooth (i.e., almost everywhere), but reduces to first order at extrema. Note that in the difference scheme of Eqs. (B.30)–(B.32), the source terms of Eq. (B.1) are integrated by using a second-order Runge-Kutta or predictor corrector explicit time-stepping procedure. This provides second-order accuracy and makes the integration of the inhomogeneous terms consistent with the Roe-method time differencing of the homogeneous terms.

Following Sweby [1984] the flux limiters $\phi_{i+1/2,k}^n$ of Eq. (B.31) are defined to be functions of the local antidiffusive flux ratios. van Leer’s flux limiter

$$
\phi_{i+1/2,k}^n = \begin{cases} 
0 & \nu_{i+1/2,k}^n > 0, b_{i,k}^n \leq 0, \\
\frac{2b_{i,k}^n}{1 + b_{i,k}^n} & \nu_{i+1/2,k}^n > 0, b_{i,k}^n > 0, \\
\frac{1}{1 + b_{i,k}^n} & \nu_{i+1/2,k}^n < 0, b_{i+1,k}^n \leq 0, \\
\frac{2}{1 + b_{i+1,k}^n} & \nu_{i+1/2,k}^n < 0, b_{i+1,k}^n > 0, 
\end{cases}
$$

(B.48)

is used for the $k = 1$ and 3 characteristic fields, and the superbee limiter of Roe

$$
\phi_{i+1/2,k}^n = \begin{cases} 
0 & \nu_{i+1/2,k}^n > 0, b_{i,k}^n \leq 0, \\
\max\left(\min(1, 2b_{i,k}^n), \min(2, b_{i,k}^n)\right) & \nu_{i+1/2,k}^n > 0, b_{i,k}^n > 0, \\
\max\left(\min(1, \frac{2}{b_{i+1,k}^n}), \min(2, \frac{1}{b_{i+1,k}^n})\right) & \nu_{i+1/2,k}^n < 0, b_{i+1,k}^n \leq 0, \\
\max\left(\min(1, 2b_{i,k}^n), \min(2, b_{i,k}^n)\right) & \nu_{i+1/2,k}^n < 0, b_{i+1,k}^n > 0, 
\end{cases}
$$

(B.49)

is used for the $k = 2$ characteristic field. The latter more compressive limiter improves the sharpness of contact surfaces. The flux ratio $b_{i,k}^n$ is given by the ratio of the antidiffusive fluxes

$$
b_{i,k}^n = \frac{|\nu_{i+1/2,k}^n|}{|\nu_{i-1/2,k}^n|},
$$

(B.50)

where $N_{U_k}$ are normalization row vectors. In the present algorithm, $N_{U_k} = [1, 0, 0]$ for $k = 1, 2, 3$.

The time-marching procedure represented by Eqs. (B.30)–(B.32)] is conditionally stable. The CFL criterion

$$
\Delta t^n < \min_i \frac{\Delta x_{i+1/2}}{|u_i^n| + a_i^n},
$$

(B.51)

is used to restrict the magnitude of the time increment and thereby ensure stability and convergence of the numerical solutions.

It is also necessary to modify the finite-difference scheme near sonic points in order
that the scheme be entropy satisfying and converge to the correct physical solution. In particular, the inviscid flux functions associated with nonlinear characteristic fields 1 and 3 must be augmented to prevent the formation of expansion shocks. A variant of the entropy fix suggested by Roe and Pike [1984] is employed. Consider elemental wave 1. A wave spreading parameter for this wave is defined to be

\[ \delta^n_{i+1/2,1} = 2[\lambda^n_{i+1/2,1} - (u^n_t - a^n_t)] . \] (B.52)

If \( \lambda^n_{i+1/2,1} - 1/2\delta^n_{i+1/2,1} < 0 \) and \( \lambda^n_{i+1/2,1} + 1/2\delta^n_{i+1/2,1} > 0 \), then the flux limiter \( \phi^n_{i+1/2,1} \) is set to zero and the first-order flux jump is split into two components; that is,

\[ \frac{1}{2}(\nu^n_{i+1/2,1} - |\nu^n_{i+1/2,1}|)\Delta U^n_{i+1/2,1} , \] (B.53)

is replaced by

\[ \frac{1}{2}(\nu^n_{i+1/2,1} - |\nu^n_{i+1/2,1}|)\Delta U^n_{i+1/2,1} + \frac{1}{2}(\nu^n_{i+1/2,1} + |\nu^n_{i+1/2,1}|)\Delta U^n_{i+1/2,1} , \] (B.54)

where

\[ \nu^n_{i+1/2,1} = \frac{1}{2}(\lambda^n_{i+1/2,1} + \frac{1}{2}\delta^n_{i+1/2,1}) , \quad \nu^n_{i+1/2,1} = \frac{1}{2}(\lambda^n_{i+1/2,1} - \frac{1}{2}\delta^n_{i+1/2,1}) . \] (B.55)

A similar procedure is required for the \( k = 3 \) nonlinear characteristic field.

**B.6.2 Solution Algorithm for Nonequilibrium Gas Flows**

For the case of the nonequilibrium thermodynamic model, Roe method solutions of Eq. (B.1) coupled with the additional species concentration and vibrational energy conservation laws of Eq. (B.15) are required. In this work, these two subsystems defining the complete solution \( U(x, t) = U(U(x, t), W(x, t)) \) are not integrated in a directly coupled simultaneous fashion. Instead, two alternate gas dynamic and thermodynamic subsystems are defined and the resulting subsystems are then integrated in a time-lagged decoupled manner. This marching algorithm may be defined as follows. Given a solution \( U(x, t_0) \) of Eqs. (B.1) and (B.15) at time \( t_0 \), an approximate solution at some later time \( t_0 + \Delta t \), where \( \Delta t \) is a small time increment, is obtained by first solving a frozen flow or gas dynamic initial value problem defined by

\[ \frac{\partial}{\partial t}(\dot{U}) + \frac{\partial}{\partial x}[F(\dot{U})] = \dot{A}(\dot{U}) + \dot{S}(\dot{U}) , \quad t_0 < t \leq t_0 + \Delta t , \] (B.56)

\[ \dot{U}(x, t_0) = \dot{U}(U(x, t_0)) = \dot{U}(U(x, t_0), W(x, t_0)) , \] (B.57)

and then solving a nonequilibrium thermodynamic initial value problem defined by

\[ \frac{\partial \dot{W}}{\partial t} + u \frac{\partial}{\partial x}[H(\dot{W})] = \dot{Q}(\dot{W}) , \quad t_0 < t \leq t_0 + \Delta t , \] (B.58)

\[ \dot{W}(x, t_0) = \dot{W}(\dot{U}(x, t_0 + \Delta t), W(x, t_0)) , \] (B.59)
where

\[
\hat{U} = \begin{bmatrix}
\rho \\
\rho u \\
\rho u^2 + p \\
\rho u (\frac{\gamma p}{(\gamma - 1) \rho} + e_v + \frac{1}{2} u^2) \\
\rho u \gamma \\
\rho u R \\
\rho u e_v
\end{bmatrix}, \quad \hat{W} = \begin{bmatrix}
c_1 \\
\vdots \\
c_N \\
c_1 e_{v1} \\
\vdots \\
c_N e_{vN} \\
\sum_{s=1}^{N} \left[ \frac{c_s R_s}{(\gamma_s - 1) T + c_s e_{v_s}} \right] + \frac{1}{2} u^2
\end{bmatrix}, \quad (B.60)
\]

\[
\hat{F} = \begin{bmatrix}
\rho u \\
\rho u^2 + p \\
\rho u (\frac{\gamma p}{(\gamma - 1) \rho} + e_v + \frac{1}{2} u^2) \\
\rho u \gamma \\
\rho u R \\
\rho u e_v
\end{bmatrix}, \quad \hat{A} = \begin{bmatrix}
-\rho u \frac{1}{A} \frac{dA}{dx} \\
-\rho u^2 \frac{1}{A} \frac{dA}{dx} \\
-\rho u (\frac{\gamma p}{(\gamma - 1) \rho} + e_v + \frac{1}{2} u^2) \frac{1}{A} \frac{dA}{dx}
\end{bmatrix}, \quad (B.61)
\]

\[
\hat{S} = \begin{bmatrix}
0 \\
F_{\text{wall}} + F_{\text{loss}} \\
Q_{\text{wall}} \\
0 \\
0 \\
0
\end{bmatrix}, \quad \hat{H} = \begin{bmatrix}
c_1 \\
\vdots \\
c_N \\
c_1 e_{v1} \\
\vdots \\
c_N e_{vN}
\end{bmatrix}, \quad \hat{Q} = \begin{bmatrix}
w_1 \\
\vdots \\
w_N \\
c_1 q_1 + \beta_1 w_1 e_{v1} \\
\vdots \\
c_N q_N + \beta_N w_N e_{vN} \\
-\sum_{s=1}^{N} w_s \Delta h_{fs}^0
\end{bmatrix}, \quad (B.62)
\]

The approximate solution at \( t_0 + \Delta t \) is then given by

\[
U(x, t_0 + \Delta t) \approx U(\hat{U}(x, t_0 + \Delta t), \hat{W}(x, t_0 + \Delta t)). \quad (B.63)
\]

A solution for all time \( t > t_0 \) may be obtained by repeating the preceding two-step algorithm and, in the limit of vanishing \( \Delta t \), this solution should converge to the exact solution of Eqs. (B.1) and (B.15).

The six-component subsystem of Eq. (B.56) has been derived by employing a frozen flow assumption and setting the finite-rate thermodynamic source terms of Eq. (B.1) to zero. Under this assumption, the behaviour of the gaseous mixture is essentially that of a
polytropic (thermally and calorically perfect) gas, except that the specific heat ratio and gas constant may vary throughout the flow field and a portion of the internal energy is locked in the vibrational modes. The last three equations of the gas dynamic subsystem are introduced to include these effects and describe changes in the quantities $\gamma$, $R$, and $e_v$, which, in the frozen flow limit, are merely convected with the flow. Note that the solution of Eq. (B.56) updates the mixture gas dynamic flow properties (e.g., $\rho$, $u$, $e$, $e_v$, $p$, etc.) but does not alter the individual species mass fractions or vibrational energies.

The multi-component $N$-species nonequilibrium thermodynamic subsystem represented by Eq. (B.58) has been derived by assuming that the velocity and density distributions are known and fixed. This set describes the time rate of change of the species mass fractions and vibrational energies and the total internal energy of the mixture. It includes the source terms neglected in the derivation of Eq. (B.58). The primitive variables $c_s$, $e_v$, and $T$, and consequently $e$, $e_v$, $p$, and the other thermodynamic properties, are all updated by solving the thermodynamic subsystem. However, $\rho$ and $u$ remain unchanged.

The preceding decoupled solution procedure is similar in spirit to the techniques put forward by Glaz et al. [1988] and Ben-Artzi [1989], and the resulting subsystems resemble the decoupled equation sets that may be obtained by using the equation-partitioning procedure suggested by Yee and Shinn [1989]. The term 'partially decoupled' is applied herein to distinguish the current method from fully-coupled algorithms, which at each level in a marching procedure solve all of the conservation equations together in a single step, and loosely-coupled or chemistry-split techniques, which at each level decouple the gas dynamic and finite-rate thermodynamic equations and solve the two sets separately in a two-stage process [Yee and Shinn, 1989].

Unlike fully-coupled methods, the present alternative provides a distinct separation of the gas dynamic and finite-rate models. As a consequence, one solver can be developed for Eq. (B.56) and used to predict the flow of many different nonequilibrium gaseous mixtures. Mixture-specific solvers are only required for Eq. (B.58). This simplifies computer program development and can make the solution algorithm more versatile than many fully-coupled techniques.

The partial-decoupling approach differs from loosely-coupled or chemistry-split methods because the decoupling procedure readily permits the use of the eigenvalues and eigenvectors of the complete system in the evaluation of the numerical fluxes of each subsystem. Loosely-coupled methods usually employ the eigenvalues and eigenvectors of each decoupled subsystem. It is believed that the use of the eigenvalues and eigenvectors of the full equations enhances the coupling between the decoupled equation sets and thereby improves numerical solution quality [Yee and Shinn, 1989].

Letting $\tilde{\mathbf{U}}_i^n$ be the numerical approximation of the solution to Eqs. (B.1) and (B.15) at $x = x_i$ and $t = t^n$, the solution at subsequent time levels is obtained by employing the partial-decoupling procedure described above and applying explicit and semi-implicit versions of Roe's method to the gas dynamic and thermodynamic subsystems, respectively. The complete algorithm can be defined by

$$
\mathbf{U}_i^{n+2} = \mathcal{L}_U^{\Delta t} \mathcal{L}_W^{2\Delta t} \mathcal{L}_U^{\Delta t} \tilde{\mathbf{U}}_i^n,
$$

(B.64)

where the solution operator $\mathcal{L}_U^{\Delta t} \mathbf{U}_i^n = \mathbf{U}((\tilde{\mathbf{U}}_i^{n+1}, \tilde{\mathbf{W}}_i^n)$ is represented by

B.18
\[
\hat{U}_{i}^{n+1} = \hat{U}_{i}^{n} + \Delta \hat{U}_{i}^{n} = \hat{U}_{i}^{n} + \Delta t^{n} \left( \hat{A}_{i}^{n} + \hat{S}_{i}^{n} \right) - \\
\frac{1}{2} \sum_{k=1}^{6} \left\{ \left( \nu_{i+1/2,k}^{n} - \nu_{i+1/2,k}^{n} \right) + \phi_{i+1/2,k}^{n} \nu_{i+1/2,k}^{n} \left( 1 - \nu_{i+1/2,k}^{n} \right) \right\} \Delta \hat{U}_{i+1/2,k}^{n} + \\
\left\{ \left( \nu_{i-1/2,k}^{n} + \nu_{i-1/2,k}^{n} \right) - \phi_{i-1/2,k}^{n} \nu_{i-1/2,k}^{n} \left( 1 - \nu_{i-1/2,k}^{n} \right) \right\} \Delta \hat{U}_{i-1/2,k}^{n} \right\} ,
\] (B.65)

\[
\bar{U}_{i}^{n+1} = \bar{U}_{i}^{n} + \Delta \bar{U}_{i}^{n} = \bar{U}_{i}^{n+1} + \frac{1}{2} \Delta t^{n} \left( \hat{A}_{i}^{n+1} - \hat{A}_{i}^{n} + \hat{S}_{i}^{n+1} - \hat{S}_{i}^{n} \right),
\] (B.66)

and the solution operator \( \mathcal{L} \hat{U}_{i}^{n} = \mathcal{U} \left( \hat{U}_{i}^{n}, \hat{W}_{i}^{n+1} \right) \) is given by

\[
\left[ I - \theta \Delta t^{n} \frac{\partial Q}{\partial W} \right]_{i} \left( \hat{W}_{i}^{n+1} - \hat{W}_{i}^{n} \right) = \left[ I - \theta \Delta t^{n} \frac{\partial Q}{\partial W} \right]_{i} \Delta \hat{W}_{i}^{n} = \Delta t^{n} \hat{Q}_{i}^{n} - \\
\frac{1}{2} \sum_{k=1}^{2N+1} \left\{ \left[ \omega_{i+1/2}^{n} - \omega_{i-1/2}^{n} \right] + \psi_{i+1/2}^{n} \omega_{i+1/2}^{n} \left( 1 - \omega_{i+1/2}^{n} \right) \right\} \Delta \mathcal{H}_{i+1/2,k}^{n} + \\
\left\{ \left[ \omega_{i-1/2}^{n} + \omega_{i-1/2}^{n} \right] - \psi_{i-1/2}^{n} \omega_{i-1/2}^{n} \left( 1 - \omega_{i-1/2}^{n} \right) \right\} \Delta \mathcal{H}_{i-1/2,k}^{n} \right\} ,
\] (B.67)

and where \( \Delta \hat{W}_{i}^{n} = \hat{U}_{i}^{n+1} - \hat{U}_{i}^{n}, \Delta \hat{U}_{i}^{n} = \hat{U}_{i}^{n+1} - \hat{U}_{i}^{n}, \Delta \hat{W}_{i}^{n} = \hat{W}_{i}^{n+1} - \hat{W}_{i}^{n}, \) and \( \hat{U}_{i}^{n+1} \), \( \hat{U}_{i}^{n+1} \), and \( \hat{W}_{i}^{n+1} \) denote intermediate solution states.

The solution of the frozen-flow gas dynamic subsystem Eq. (B.56) is provided by the difference scheme of Eqs. (B.65) and (B.66). As was the case for the solution of the hyperbolic conservation laws of gases obeying the ideal and equilibrium real-gas equations of state, the quantities \( \nu_{i+1/2,k}^{n} \) and \( \Delta \bar{U}_{i+1/2,k}^{n} \) appearing in these equations are again the local average CFL numbers and solution jump vectors. They are defined in terms of the eigenvalues and eigenvectors \( \lambda_{i+1/2,k}^{n} \) and \( e_{i+1/2,k}^{n} \) of the Jacobian matrix \( \mathbf{J} = \frac{\partial \mathbf{F}}{\partial \mathbf{U}} \) evaluated at some average state and are given by

\[
\nu_{i+1/2,k}^{n} = \frac{\Delta t^{n} \lambda_{i+1/2,k}^{n}}{\Delta x_{i+1/2}},
\] (B.68)

\[
\Delta \hat{U}_{i+1/2,k}^{n} = \alpha_{i+1/2,k}^{n} e_{i+1/2,k}^{n},
\] (B.69)

where \( \alpha_{i+1/2,k}^{n} \) are the wave strengths. It can be shown that the eigenvalues and eigenvectors of the flux Jacobian \( \mathbf{J} \) of the six-component subsystem represented by Eq. (B.56) are

\[
\lambda_{i+1/2,1}^{n} = u_{i+1/2}^{n} - a_{i+1/2}^{n}, \quad \lambda_{i+1/2,2}^{n} = u_{i+1/2}^{n} + a_{i+1/2}^{n},
\] (B.70)

\[
\lambda_{i+1/2,3}^{n} = \lambda_{i+1/2,4}^{n} = \lambda_{i+1/2,5}^{n} = u_{i+1/2}^{n},
\] (B.71)
\[ e_{i+1/2,1}^n = \begin{bmatrix} \frac{1}{2} (u_{i+1/2}^n - a_{i+1/2}^n) \\ \gamma_{i+1/2}^n - u_{i+1/2}^n a_{i+1/2}^n \\ R_{i+1/2}^n \\ e_{v_{i+1/2}}^n \end{bmatrix}, \quad e_{i+1/2,6}^n = \begin{bmatrix} \frac{1}{2} (u_{i+1/2}^n + a_{i+1/2}^n) \\ \gamma_{i+1/2}^n + u_{i+1/2}^n a_{i+1/2}^n \\ R_{i+1/2}^n \\ e_{v_{i+1/2}}^n \end{bmatrix}, \quad (B.72) \]

\[ e_{i+1/2,2}^n = \begin{bmatrix} \frac{1}{2} (u_{i+1/2}^n)^2 + e_{v_{i+1/2}}^n \\ \gamma_{i+1/2}^n \\ R_{i+1/2}^n \\ e_{v_{i+1/2}}^n \end{bmatrix}, \quad e_{i+1/2,3}^n = \begin{bmatrix} 0 \\ 0 \\ -\frac{(a_{i+1/2}^n)^2}{(\gamma_{i+1/2}^n - 1)^2} \\ 0 \end{bmatrix}, \quad (B.73) \]

\[ e_{i+1/2,4}^n = \begin{bmatrix} 0 \\ 0 \\ 0 \\ R_{i+1/2}^n \\ 0 \end{bmatrix}, \quad e_{i+1/2,5}^n = \begin{bmatrix} 0 \\ 0 \\ e_{v_{i+1/2}}^n \\ 0 \\ e_{v_{i+1/2}}^n \end{bmatrix}, \quad (B.74) \]

with \( h = [\gamma p/(\gamma - 1)\rho] + e_v + u^2/2 \). An extension of Roe's approximate Riemann solver has been developed herein to specify the appropriate average state primitive variables and wave strengths used in the preceding equations. This extension of the approximate Riemann problem solution for the subsystem of Eq. (B.56) yields the following approximations for the averages:

\[ \rho_{i+1/2}^n = \sqrt{\rho_{i+1}^n \rho_i^n}, \quad (B.75) \]

\[ Z_{i+1/2}^n = \frac{\sqrt{\rho_{i+1}^n Z_{i+1}^n} + \sqrt{\rho_i^n Z_i^n}}{\sqrt{\rho_{i+1}^n} + \sqrt{\rho_i^n}}, \quad Z = u, \gamma, R, e_v, \text{ and } h, \quad (B.76) \]

\[ a_{i+1/2}^n = \left\{ (\gamma_{i+1/2}^n - 1) \left[ h_{i+1/2}^n - e_{v_{i+1/2}}^n - \frac{1}{2} \left( u_{i+1/2}^n \right)^2 \right] \right\}^{1/2}, \quad (B.77) \]

and wave strengths

\[ \alpha_{i+1/2,1}^n = \frac{1}{2(a_{i+1/2}^n)^2} \left[ \Delta p_{i+1/2}^n - \rho_{i+1/2}^n a_{i+1/2}^n \Delta u_{i+1/2}^n \right], \quad (B.78) \]
Note that the flux limiters \( \phi_{i+1/2,k} \), which provide the difference scheme of Eqs. (B.65) and (B.66) with the desirable TVD property, are evaluated similarly to the limiters used in the solution for the polytropic and equilibrium cases. The flux limiter of van Leer defined by Eq. (B.48) is used for the \( k = 1 \) and \( 6 \) characteristic fields and the superbee flux limiter of Eq. (B.49) is used for the \( k = 2, 3, 4, \) and \( 5 \) characteristic fields. Appropriate values for the flux ratios and normalization row vectors are used. Finally, note also that the flux functions of the \( k = 1 \) and \( 6 \) nonlinear characteristic fields are modified by employing entropy fixes of the form given by Eqs. (B.52)-(B.55).

The integration of the thermodynamic subsystem Eq. (B.58) is provided by the TVD semi-implicit scheme of Eq. (B.67). In Eq. (B.67), \( I \) is the identity matrix, \( \partial \mathbf{Q} / \partial \mathbf{W} \) is the source Jacobian matrix, \( \omega_{i+1/2}^n \) and \( \Delta \mathbf{H}_{i+1/2,k}^n \) are the local average CFL number and solution jump vectors used in evaluating the flux functions for the species concentration and vibrational energy equations, and \( \psi_{i+1/2,k}^n \) are the flux limiters. The homogeneous form of the subsystem given by Eq. (B.58) is essentially a system of independent convection equations and, therefore, the numerical flux functions can be evaluated quite simply. The CFL number \( \omega_{i+1/2}^n \) is given by

\[
\omega_{i+1/2}^n = \frac{\Delta t^n u_{i+1/2}^n}{\Delta x_{i+1/2}},
\]

where \( u_{i+1/2}^n \) is evaluated by using Eqs. (B.75) and (B.76) arising from the extended approximate Riemann problem solution. This ensures that the eigenvalues and eigenvectors of the fully-coupled system are used in the computation of the flux functions of both the gas dynamic and thermodynamic subsystems. The solution jump column vectors for the \( ND = 2N + 1 \) component thermodynamic subsystem are given by

\[
\Delta \mathbf{H}_{i+1/2,k}^n = \mathbf{D}_k \Delta \mathbf{H}_{i+1/2,k}^n,
\]

where \( \Delta \mathbf{H}_{i+1/2,k}^n = \mathbf{H}_{i+1}^p - \mathbf{H}_i^p \), \( \mathbf{D}_k \) is a diagonal matrix for which the elements of the diagonal are \( (\delta_{1k}, \ldots, \delta_{kk}, \ldots, \delta_{N_D,k}) \), and \( \delta \) is the usual Kronecker delta function. Finally, the flux limiters \( \psi_{i+1/2,k}^n \) for each component of the solution vector, which limit the magnitude of the antidiffusive flux in Eq. (B.67), are evaluated by employing the superbee formulation of Eq. (B.49). The flux ratio is again defined in terms of the ratio and the antidiffusive fluxes and the normalization row vector is chosen to recover the component of the antidiffusive flux vector associated with the \( k \)th component of the solution vector \( \mathbf{W} \). Note that entropy corrections are not required in the solution of the thermodynamic subsystem.

The stiffness of the source terms associated with the finite-rate reaction and relaxation
processes of Eq. (B.67) force the time step sizes of explicit schemes to be excessively small and the corresponding computer times to be prohibitively large. For this reason, the source terms of the operator \( L^{At} \) are integrated by using an implicit time-stepping procedure that is similar to the semi-implicit algorithms proposed by Bussing and Murman [1988], Yee and Shinn [1989], and Ben-Artzi [1989] for the computation of chemically reacting flows. These schemes treat only the source terms implicitly. This effectively alleviates the stiffness associated with the finite-rate relaxation and reaction time scales while avoiding large matrix inversions. The quantity \( [I - \theta \Delta t^n (\partial Q/\partial W)^T] \) is similar to the preconditioning matrices used by Bussing and Murman [1988]. The parameter \( \theta \) controls the implicit time stepping. For \( \theta = 0 \), the time differencing is Euler explicit. For \( \theta = 1 \), the time differencing is Euler implicit. This value produces the most stable scheme and is appropriate for problems with extremely stiff source terms. A value of \( \theta = 1/2 \) produces a trapezoidal implicit time differencing that is best suited and consistent with the explicit time-differencing of the homogeneous terms. Note that the time-marching procedure represented by Eqs. (B.64)–(B.67) is conditionally stable. For \( \theta \geq 1/2 \), the CFL condition Eq. (B.51) ensures stability and convergence.

### B.6.3 Boundary Conditions

Boundary conditions are necessary for the prescription of the numerical solutions at the extremities of the computational domains. There are two types of boundary conditions required for the hypersonic impulse tunnel simulations. Firstly, a solid-surface reflecting boundary condition is needed for the flow properties at the closed end of the reservoir and the front and back faces of the moving piston. Secondly, an outflow boundary condition is needed for the flow properties at the exit of the contoured nozzle.

Reflecting boundary conditions are applied by forcing the flow to have the velocity of the solid boundary or piston and then employing Rankine-Hugoniot and Riemann invariant relations across shocks and rarefaction waves to determine the other solution properties. For the outflow boundary condition at the nozzle exit, it is recognized that, except for very early in the tunnel operation cycle, the flow is almost always supersonic at this point and disturbances from the test section cannot propagate upstream. Simple constant extrapolation or transmissive boundary conditions [Kamowitz, 1988] at the nozzle exit are therefore quite appropriate and are used here.

### B.7 Numerical Results and Performance Data

This section presents numerical predictions of the UTIAS-RPI hypersonic impulse tunnel performance obtained by solving the one-dimensional flow and thermodynamic model equations of Sections 3 and 4 using the TVD numerical integration schemes described in Section 5. The performance of the facility is first assessed by considering its operation under two firing states that are commonly used for much of the ongoing experimental hypersonic research at UTIAS. Additional numerical results are then presented to establish more thoroughly the tunnel performance envelope and operating range.

The UTIAS-RPI impulse tunnel is generally operated with initial reservoir pressure \( p_{res} = 20.5 \) MPa, initial reservoir and barrel temperatures \( T_{res} = T_{brl} = 293 \) K, and piston mass \( m_p = 96 \) g. Different operating conditions are achieved by varying the initial barrel pressure \( p_{brl} \). Two firing modes are employed in the majority of experiments. In one mode,
\( p_{brl} = 400 \text{ kPa} \) and in the other, \( p_{brl} = 200 \text{ kPa} \). Note that the firing state with the lower initial barrel pressure produces a higher stagnation enthalpy flow in the test section.

For the computations of the tunnel operation in these two modes, and indeed for all of the predictions presented in this section, the unsteady motion of the driver and working gases is solved for the entire facility between the closed end of the reservoir and the nozzle exit. The cross-sectional area function \( A(x) \) used in the numerical simulations is illustrated in Figure B.2 in terms of the axial position \( x \) and local tunnel radius \( r(x) \) where \( A = \pi r^2 \). A total of 570 spatial nodes are used to represent the discretized computational domain. Convergence tests suggest that this nodal density is sufficient as numerical errors appear to be nominally less than 3–5% when 500–600 nodes are used. Boundary-layer frictional losses and heat transfer are included with \( \varepsilon = 0.025 \text{ mm} \). These loss effects are, however, not included in the computation of the flow in the nozzle section. This is a reasonable approximation because the flow in this section of the tunnel is definitely not fully developed. The nozzle has been specifically designed to produce a relatively large inviscid core flow with a boundary layer that is confined, for the most part, to the near wall region. A value of 0.25 is assumed for the head-loss coefficients \( K \) of the two diaphragms located just downstream of the ball valve section. Note that the diaphragm head losses are phased in during the first 5 ms after diaphragm rupture using a linear-ramping function in order to more accurately simulate the developing flow situation occurring in the initial stages of tunnel startup. All of the computations were performed on a Hewlett-Packard/Apollo 400s workstation. The simulations of the ideal and equilibrium gas cases required approximately 4–5 central-processing-unit (CPU) hours, whereas the nonequilibrium gas cases required about 13–14 CPU hours.

The predictions of the tunnel operation with initial barrel pressures of 400 and 200 kPa are presented in Figures B.3–B.14. The first set of results for a barrel pressure of 400 kPa is given in Figures B.3–B.7, whereas the other set for a barrel pressure of 200 kPa is in Figures B.8–B.14. Note that the calculations were performed with the ideal, real equilibrium, and five-species four-temperature nonequilibrium gas models, and the results for these three different thermodynamic models are compared in these figures.

Consider first the results with \( p_{brl} = 400 \text{ kPa} \). The piston velocity \( V_p \) and acceleration \( a_p \) as a function of piston position in the barrel \( x_p \) are given in Figure B.3. From the figure, it is clear that the piston rapidly accelerates during the first metre of travel and then is subjected to very little acceleration until the first reflected shock from the barrel end causes it to decelerate. Subsequent reflections cause further deceleration and the piston eventually comes to rest at the end of the barrel \( (x_p \approx 6.7 \text{ m}) \). A maximum velocity of somewhere near 515 m/s and a peak acceleration approaching 760 km/s\(^2\) are predicted. The figure also clearly illustrates that high-temperature and (or) real-gas effects have very little effect on the predicted piston motion. The piston trajectories determined using the real equilibrium and nonequilibrium gas thermodynamic models are virtually identical to the trajectory obtained using the polytropic model.

The predicted temporal variations of the stagnation pressure \( p_o \) and temperature \( T_o \) at the end of the barrel as the flow in the nozzle relaxes towards a steady state condition are illustrated in Figures B.4 and B.5. The time \( t = 0 \), in these and other temporal distributions to follow, corresponds to the time when the first of the two diaphragms ruptures. The multiple shock reflections associated with the nonisentropic compression of the working gas is clearly illustrated by the successive pressure and temperature jumps in the time histories. These jumps indicate the passage of the reflected shocks between the piston front face and end of the barrel. The two sets of curves in the figures indicate that high-temperature phe-
nomena are important in determining the nozzle flow stagnation conditions. Although there are only minor differences between the ideal, equilibrium, and nonequilibrium results for the stagnation pressures, the stagnation temperatures obtained with each thermodynamic model are quite different. It can be seen that the predicted stagnation pressure during the period of relatively steady-state nozzle flow is between 24–27 MPa for all three thermodynamic models. This pressure begins to drop rapidly around \( t = 39 \) ms when the working gas is depleted and the piston comes to rest at the end of the barrel. The polytropic model provides a higher stagnation temperature than the temperatures predicted by the two real-gas models, as should be expected. The predicted ideal stagnation temperature appears to be around 980–1000 K whereas the equilibrium and nonequilibrium values are around 910–920 and 940–950 K, respectively. Note that at these stagnation temperatures, vibrational excitation of the nitrogen (\( \text{N}_2 \)) and oxygen (\( \text{O}_2 \)) diatomic molecules is significant, but dissociation of these species is small. The differences in the curves of Figure B.5 indicate that nonequilibrium relaxation must be considered in order to determine the stagnation temperature accurately.

As an additional comparison, an experimental stagnation pressure trace measured during a firing of the UTIAS-RPI facility with an initial barrel pressure of 400 kPa is also presented in Figure B.4. It is evident from the figure that many of the detailed features and complicated wave structure of the nonstationary flow in the tunnel, such as shock strengths and times of arrival, are correctly reproduced by the one-dimensional nonstationary flow model calculations and that the numerical predictions are in good agreement with the experimental time-history data, both qualitatively and quantitatively.

Figure B.6 depicts the temporal variation of the flow Mach number \( M_a \) at the exit of the contoured nozzle. The figure clearly demonstrates the establishment of steady flow in the nozzle. The exit Mach number initially oscillates about a mean value. These oscillations indicate the passage of transmitted shock waves through the nozzle and test section. A relatively steady-state nozzle flow is then achieved at about 25 ms after the first diaphragm has burst and is maintained until sometime just after the \( t = 40 \) ms mark. At this time, the piston has come to rest and the stagnation pressure and temperature at the nozzle entrance have dropped dramatically. This suggests a run time of somewhere between 15 and 17 ms for this particular mode of tunnel operation. It is interesting to note that, as mentioned in Section 2, the contoured nozzle employed in the present impulse tunnel configuration was built with an exit flow Mach number of 8.33 as one of the design specifications and that, for all thermodynamic models, the predicted steady-state nozzle exit Mach number is about 8.35–8.45. Note also that the numerical results show that the pressure \( p \), temperature \( T \), and specific heat ratio \( \gamma \) of the air flow at the nozzle exit are approximately 1.6–1.7 kPa, 65–75 K, and 1.4, respectively.

Plots of the spatial distributions of the vibrational temperatures of the two excited diatomic species (\( \text{N}_2 \) and \( \text{O}_2 \)) and the equilibrium translational and rotational temperature at time \( t = 30 \) ms in the UTIAS-RPI tunnel from the piston front face to nozzle exit are also shown in Figure B.7. These numerical results were obtained with the nonequilibrium thermodynamic model. Note that the calculations performed show that in this operation mode dissociation/recombination effects are negligible and the principal nonequilibrium phenomenon that occurs at stagnation in the barrel is vibrational relaxation. This is as expected for these stagnation temperatures. It has long been known that typically vibrationally excited air freezes when it becomes moderately supersonic [Stollery and Smith, 1962; Stollery and Park, 1963] and this seems to be the case here. The distributions of Figure B.7 demonstrate that the air in the nozzle freezes somewhere close to the nozzle throat, with the
nitrogen freezing first near 965 K and the oxygen following at a temperature of about 620 K. This produces a test-section air flow with excited vibrational energy states and vibrational temperatures much higher than the equilibrium translational-rotational temperature of 67 K.

Figures B.8–B.12 show the numerical predictions of the UTIAS-RPI hypersonic impulse tunnel operation with an initial barrel pressure of 200 kPa. The results are similar to those of the 400 kPa simulations, except that the maximum piston velocity is now higher and approaches 600 m/s, the stagnation pressure is around 24–25 MPa, the simulated stagnation temperatures are considerably higher ranging from 1070–1210 K, and the duration of steady nozzle flow is now reduced to about 9.5 ms. Figure B.9 illustrates that, except for some differences in the later stages of the tunnel operation cycle (t > 30 ms), the agreement between numerical predictions and experimental measurements of the stagnation pressure is again good. The differences after t = 30 ms can be explained as follows. The stagnation pressure ahead of the piston drops in the numerical predictions. However, this characteristic pressure drop is not observed in the experimental signature because, in this particular firing, the piston has passed by the transducer and sealed the entrance to the nozzle. Figure B.12 provides further evidence that the air flow at the nozzle exit, and thus the air flow in the test section, of the UTIAS-RPI facility has considerable energy locked in the excited vibrational modes of the nitrogen and oxygen gas molecules. Vibrational temperatures at the nozzle exit of 1180 and 830 K are predicted for N₂ and O₂, respectively. Note that the low-amplitude oscillatory nature of the N₂ temperature distribution of Figure B.12 in the region downstream of the throat is a consequence of the temporal variations in the stagnation conditions created by the nonisentropic compression process occurring in the barrel.

Two additional results are given for this second set of predictions with an initial barrel pressure of 200 kPa. Shown in Figures B.13 and B.14 are the temporal variation of the static pressure and temperature at the nozzle exit as calculated using the three thermodynamic models (ideal, real equilibrium, and five-species four-temperature nonequilibrium gas models). These two figures clearly depict the rather unsteady nature of the flow that is present at the nozzle exit (and thus in the test section) during gun tunnel operation.

Before continuing, it is worth mentioning that the influence of boundary-layer friction and heat-transfer, included in the present analysis, are important and cannot be neglected if accurate predictions of stagnation, nozzle, and test-section flow properties are desired. This is illustrated in Figure B.15, where two predictions of the ideal-gas stagnation pressure p₀ are depicted. In one case the stagnation pressure is computed with the boundary-layer losses included and in the other these effects have been omitted. It is apparent that the times of arrival and strengths of nonstationary shocks, as well as the resulting steady-state stagnation pressure, are very different for these two cases. In order to obtain the level of quantitative agreement between numerical predictions and experimental measurements found in Figures B.4 and B.9, the incorporation of boundary-layer effects into the analysis seems to be required.

It should also be noted that the time scales associated with the finite-rate source terms in the preceding nonequilibrium computations were approximately 500–10,000 times smaller than the gas dynamic time scales. The semi-implicit solver of Eqs. (B.64)–(B.67) effectively removed the stability constraints imposed by the finite-rate times scales and permitted the computations to be performed with the numerical time steps controlled only by the gas dynamic time scales.

The performance characteristics of the UTIAS-RPI hypersonic impulse tunnel are fur-
ther illustrated by the numerical results depicted in Figures B.16–B.21. In these figures, the computed barrel end stagnation pressure $T_o$, facility run time $\Delta t$, nozzle exit flow Mach number $Ma$, and nozzle exit flow Reynolds number per unit length $Re/L$ are given as functions of the initial barrel pressure $p_{brl}$, piston mass $m_p$, and initial barrel temperature $T_{brl}$. The results are again given for all three thermodynamic models.

In Figures B.16–B.19, the effects of varying the initial barrel pressure from 100 to 800 kPa with $p_{res} = 20.5$ MPa, $T_{res} = T_{brl} = 293$ K, and $m_p = 96$ g all fixed are explored. Figure B.16 shows that by reducing the barrel pressure higher stagnation temperatures approaching 1500 K are possible. However, Figure B.17 shows that these moderate increases in stagnation enthalpy are offset by a corresponding decrease in the facility run time, which may be detrimental to experiments in many cases. Note that the run times are virtually the same for all three thermodynamic models. Figure B.18 illustrates that the test-section flow Mach number is rather insensitive to the initial barrel pressure. This should be expected for it depends primarily on the exit to throat area ratio. Although not shown, the stagnation pressure was also found to be insensitive to initial barrel pressure. Values for $p_o$ were found to be around 24–27 MPa for all of the operating conditions considered. Finally, Figure B.19 presents the range of nozzle-exit or test-section flow Reynolds number per unit length that may be achieved with the UTIAS-RPI tunnel. The Reynolds number varies from $10^7$ to $5 \times 10^7$ m$^{-1}$, which suggests that, depending on the model size and orientation in the test section, fully laminar, transitional, and even fully turbulent boundary-layers may be obtained.

For many experimental programs, higher test-section stagnation temperatures are desired. Two of the possible and more practical avenues for achieving higher temperatures are to re-design and reduce the piston mass by employing lightweight high strength materials or to preheat the working gas in the barrel before diaphragm rupture. The effects of varying the piston weight and initial barrel temperature with $p_{res} = 20.5$ MPa, $T_{res} = 293$ K, and $p_{brl} = 200$ and 400 kPa are shown in Figures B.20 and B.21. It should be obvious from Figure B.20 that changing the piston mass has little effect. Even the reduction of the piston mass by as much as 75% provides a corresponding increase in the predicted stagnation temperatures of only 40 K. On the other hand, Figure B.21 shows that preheating the barrel gases is more worthwhile. An increase in the initial barrel temperature of 200 K can provide a corresponding increase in the stagnation pressure of up to 400 K. It should, however, be noted that preheating the working gas does reduce the run time. With $p_{brl} = 200$ kPa, the run time $\Delta t$ was found to decrease almost linearly with temperature from about 10 ms at $T_{brl} = 293$ K down to 5 ms at $T_{brl} = 750$ K.

## B.8 Concluding Remarks

A quasi-one-dimensional unsteady flow analysis and TVD finite-difference solution algorithm with new numerical features have been presented for the prediction of the UTIAS-RPI hypersonic impulse tunnel operation and performance. Unlike previous studies which have generally employed quasi-steady and mostly analytic techniques, modern CFD methods are used to predict for the first time the complete unsteady behaviour of the impulse tunnel from initial startup to blow down. Furthermore, the use of polytropic gas, real equilibrium gas, and four-temperature five-species nonequilibrium gas thermodynamic models in the analysis has permitted the evaluation of high temperature effects for this experimental facility. Numerical results and comparisons to available experimental data have demonstrated
the capabilities and usefulness of these modeling techniques.

Under typical operating conditions, the numerical predictions have shown that the run time for the UTIAS-RPI impulse tunnel is about 15–20 ms and that the stagnation pressure and temperature are 24–27 MPa and 1000–1200 K, respectively. Test section flow Mach and Reynolds numbers of 8.35–8.45 and $10^7$ to $5 \times 10^7$ m$^{-1}$ were found. In addition, the static pressure and temperature in the test section were determined to be about 1.6–1.7 kPa and 65–75 K, respectively. For the predicted stagnation enthalpies, it was shown that in most cases the primary high-temperature phenomenon occurring in the tunnel was vibrational excitation. The degrees of dissociation of $N_2$ and $O_2$ were found not to exceed 1/2 and 2%, respectively, even in the extreme cases considered where stagnation temperatures neared 2000 K. It was also demonstrated that vibrational excitation must be treated as a finite-rate process to obtain accurate predictions of the tunnel stagnation conditions.

Vibrational relaxation effects were also found to be of importance in the hypersonic nozzle flows of the UTIAS-RPI facility. It was shown that the air typically freezes downstream but very close to the nozzle throat and results in test-section flows with nitrogen and oxygen species having vibrational temperatures of 960–1200 K and 620–830 K, respectively. These temperatures are much higher than the predicted test-section translational-rotational temperatures and may be important in the assessment of tunnel experimental data.

One of the limitations of the UTIAS-RPI facility seems to be the rather low stagnation enthalpies that can be obtained. The present performance assessment of the impulse tunnel indicates a possible technique for extending the range of flow conditions that can be achieved in the test section. Reducing the piston weight proves to be fruitless; however, preheating of the working gas can lead to substantially higher stagnation temperatures and feasible preheating mechanisms could be examined in the future.
Figure B.1: UTIAS-RPI hypersonic impulse tunnel.
(a) Schematic diagram of facility,
(b) $x$-$t$ diagram of tunnel operation.

Figure B.2: UTIAS-RPI hypersonic impulse tunnel geometry
used in numerical simulations.
Figure B.3: Piston velocity $V_p$ and acceleration $a_p$, $p_{res} = 20.5$ MPa, $p_{brl} = 400$ kPa, $T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.

Figure B.4: Barrel end stagnation pressure $p_o$, $p_{res} = 20.5$ MPa, $p_{brl} = 400$ kPa, $T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.
Figure B.5: Barrel end stagnation temperature $T_o$,
$p_{res} = 20.5$ MPa, $p_{brl} = 400$ kPa,
$T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.

Figure B.6: Nozzle exit Mach number $M_a$,
$p_{res} = 20.5$ MPa, $p_{brl} = 400$ kPa,
$T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.
Figure B.7: Temperature distributions in nozzle, $t = 30$ ms, $p_{res} = 20.5$ MPa, $p_{brl} = 400$ kPa, $T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.
Figure B.8: Piston velocity $V_p$ and acceleration $a_p$,
$p_{res} = 20.5$ MPa, $p_{bri} = 200$ kPa,
$T_{res} = T_{bri} = 293$ K, $m_p = 96$ g.

Figure B.9: Barrel end stagnation pressure $p_o$,
$p_{res} = 20.5$ MPa, $p_{bri} = 200$ kPa,
$T_{res} = T_{bri} = 293$ K, $m_p = 96$ g.
Figure B.10: Barrel end stagnation temperature $T_o$,
$p_{res} = 20.5$ MPa, $p_{brl} = 200$ kPa,
$T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.

Figure B.11: Nozzle exit Mach number $M_a$,
$p_{res} = 20.5$ MPa, $p_{brl} = 200$ kPa,
$T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.
Figure B.12: Temperature distributions in nozzle, $t = 30$ ms,
$p_{res} = 20.5$ MPa, $p_{brl} = 200$ kPa,
$T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.
Figure B.13: Nozzle exit static pressure $p$,
$p_{res} = 20.5 \text{ MPa}, p_{brl} = 200 \text{ kPa},$
$T_{res} = T_{brl} = 293 \text{ K}, m_p = 96 \text{ g}.$

Figure B.14: Nozzle exit static temperature $T$,
$p_{res} = 20.5 \text{ MPa}, p_{brl} = 200 \text{ kPa},$
$T_{res} = T_{brl} = 293 \text{ K}, m_p = 96 \text{ g}.$
Figure B.15: Barrel end stagnation pressure $p_o$,
$p_{res} = 20.5$ MPa, $p_{brl} = 400$ kPa,
$T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.
Figure B.16: Barrel end stagnation temperature $T_o$ as a function of initial barrel pressure $p_{brl}$, $p_{res} = 20.5$ MPa, $T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.

Figure B.17: Run time $\Delta t$ as a function of the initial barrel pressure $p_{brl}$, $p_{res} = 20.5$ MPa, $T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.
Figure B.18: Nozzle exit Mach number $M$ as a function of initial barrel pressure $p_{brl}$, $p_{res} = 20.5$ MPa, $T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.

Figure B.19: Nozzle exit Reynolds number per unit length $R/L$ as a function of the initial barrel pressure $p_{brl}$, $p_{res} = 20.5$ MPa, $T_{res} = T_{brl} = 293$ K, $m_p = 96$ g.
Figure B.20: Barrel end stagnation temperature $T_o$ as a function of the piston mass $m_p$, $p_{res} = 20.5$ MPa, $p_{brl} = 200 \& 400$ kPa, $T_{res} = T_{brl} = 293$ K.

Figure B.21: Barrel end stagnation temperature $T_o$ as a function of initial barrel temperature $T_{brl}$, $p_{res} = 20.5$ MPa, $p_{brl} = 200 \& 400$ kPa, $T_{res} = 293$ K, $m_p = 96$ g.
Appendix C

Nonequilibrium Thermodynamic Model for Air

C.1 Summary

A five-species (N₂, O₂, NO, N, and O) four-temperature (i.e., translational-rotational temperature \( T \), and vibrational energies \( e_{vN₂}, e_{vO₂}, \) and \( e_{vNO} \)) thermochemical nonequilibrium model for air is described suitable for inviscid continuum flow calculations. In the multivibrational-temperature nonequilibrium model, the chemical reaction mechanism of air is represented by seventeen elementary reactions, fifteen dissociation/recombination reactions and two exchange reactions. A Landau-Teller harmonic oscillator formulation is used to model the vibrational nonequilibrium rate or relaxation processes. Chemical-vibrational coupling and ionization effects are neglected. The various physical assumptions, model equations, rate constants, and parameters, as well as model limitations, are discussed. This five-species four-temperature model is valid for temperatures up to 8,000 K and can be used to represent the flows of either pure oxygen and nitrogen by setting the mass concentrations of the other species to zero.

C.2 Introduction

For the purposes of the present numerical study concerning thermochemical nonequilibrium flow prediction (refer to Chapters 3 and 4 of the main text for a complete description of the flow equations of interest and proposed total-variation-diminishing flux-difference split solution algorithms), the high-speed gases are modeled by treating them as a chemically reactive thermally perfect mixture. The thermal state of the mixture is described by a translational-rotational temperature and a set of vibrational temperatures, one for each polyatomic species. Neglecting ionization rate processes and radiation effects and confining ourselves to inviscid continuum flows, the weakly conservative forms of the mixture mass, momentum, and energy equations, as well as species mass and vibrational energy equations, governing the gaseous flow may be written for a general Cartesian coordinate system using the usual tensor notation as [Vincenti and Kruger, 1975; Anderson, 1982; Anderson, 1989; Gnoffo et al., 1989]

\[
\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_i}(\rho u_i) = 0, \tag{C.1}
\]

\[
\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j + \delta_{ij}p) = 0, \tag{C.2}
\]
\[
\frac{\partial}{\partial t} \left[ \rho (e_{tr} + e_v + \frac{1}{2} u_i u_i) \right] + \frac{\partial}{\partial x_j} \left[ \rho u_j (e_{tr} + \frac{p}{\rho} + e_v + \frac{1}{2} u_i u_i) \right] = -\rho \sum_{s=1}^{N} w_s \Delta h^0_s, \quad (C.3)
\]
\[
\frac{\partial}{\partial t} (\rho c_s) + \frac{\partial}{\partial x_i} (\rho c_s u_i) = \rho w_s, \quad s = 1, \ldots, N, \quad (C.4)
\]
\[
\frac{\partial}{\partial t} (\rho c_s e_{v_s}) + \frac{\partial}{\partial x_i} (\rho c_s e_{v_s} u_i) = \rho c_s q_s + \rho \beta_s w_s e_{v_s}, \quad s = 1, \ldots, N. \quad (C.5)
\]

In Equations (C.1)-(C.5), \( t \) is time, \( x_i \) are the Cartesian coordinates, and \( \delta_{ij} \) is the Kronecker delta function. Additionally, \( \rho \) is the mixture density, \( u_i \) is the \( i \)-direction velocity, \( p \) is the total pressure of the mixture (i.e., sum of the partial pressures), \( e_{tr} \) is the total specific translational-rotational energy of the mixture, \( c_s = \rho_s / \rho \) is the mass fraction of species \( s \) with \( \sum_s c_s = 1 \), \( \rho_s \) is the density of species \( s \), \( e_{v_s} \) is the specific vibrational energy of species \( s \), \( e_v = \sum_s c_s e_{v_s} \) is the total specific vibrational energy of the mixture, and \( N \) is the number of species in the mixture. The quantity \( \Delta h^0_s \) is defined to be the heat of formation of species \( s \) and the source term \( -\rho \sum w_s \Delta h^0_s \) of Eq. (C.3) represents the total change in the zero-point energy of the mixture resulting from the finite-rate chemical processes. The variable \( w_s \) represents the time rate of change of the species concentrations due to the chemical reactions, whereas \( q_s \) is the time rate of change of the vibrational energy of the species \( s \) brought about by the vibrational relaxation processes. Finally, the term \( \rho \beta_s w_s e_{v_s} \) appearing in Eq. (C.5) models the change in the vibrational energy of species \( s \) per unit volume of the mixture due to the chemical reactions, where \( \beta_s \) is an empirical value greater than or equal to unity that is used to reflect the observed preference of higher-than-average vibrationally excited molecules to dissociate and the tendency of atoms to combine and form higher-than-average vibrationally excited molecules [Gnoffo et al., 1989].

The numerical solution of the preceding partial-differential equations (PDEs) requires the prescription of the inhomogeneous source terms (i.e., \( q_s \) and \( w_s \)) which, in turn, necessitate a detailed modeling of the finite-rate vibrational relaxation and chemical reaction processes for the gaseous mixture under consideration. For the simulation of hypersonic flight in the earth’s atmosphere, nonequilibrium modeling for air is required. Described herein is a five-species four-temperature thermochemical nonequilibrium model suitable for inviscid continuum air flow calculations. The five species considered are diatomic nitrogen, oxygen, and nitric oxide (\( \text{N}_2, \text{O}_2, \text{and NO} \)), and monatomic nitrogen and oxygen (\( \text{N} \) and \( \text{O} \)). The four temperatures or energies used to describe the partitioning of the internal energy among the various energy states of the air molecules and atoms are the equilibrium translational-rotational temperature \( T \), and vibrational energies of the three diatomic species \( e_{v_{\text{N}_2}}, e_{v_{\text{O}_2}}, \) and \( e_{v_{\text{NO}}} \). In this model, the chemical reaction mechanism of air is represented by seventeen elementary reactions. A Landau-Teller harmonic oscillator formulation is used to model the vibrational relaxation processes and chemical-vibrational coupling effects are not included. The thermodynamics model uses established rate data and is quite similar to the finite-rate model employed by Glaz et al. [1988] for the computation of oblique shock-wave reflections. Although other, possibly more sophisticated, models for air that involve greater numbers of species are used in other nonequilibrium flow studies (e.g., [Park, 1988; Park, 1989; Gnoffo et al., 1989; Mitcheltree, 1991; Sagnier and Marraffa, 1991]), the proposed five-species four-temperature model should be quite accurate for temperatures up to perhaps 8,000 K and pressures above about 0.10 kPa [Vincenti and Kruger, 1975]. For temperatures above 8,000 K, ionization and other rate processes become significant and eleven-species models (five neutral species \( \text{N}_2, \text{O}_2, \text{NO}, \text{N}, \) and \( \text{O} \), five ions \( \text{N}_2^+, \text{O}_2^+, \text{NO}^+ \), ...
N\(^+\), and O\(^+\), and free electrons e\(^-\)) are required to describe the chemical composition of ionized air when temperatures exceed 9,000 K [Anderson, 1989].

The remainder of the appendix is devoted to providing a complete description of the five-species nonequilibrium thermodynamic model for air. Details of the rate equations used to model the chemical and vibrational finite-rate processes are given and correlations for various reaction rate coefficients and relaxation times are provided, along with the accompanying physical constants and data. Some limitations and possible extensions of the model are also discussed.

Before continuing, it should be mentioned that the present four-temperature model for air differs conceptually from two- and three-temperature models, summaries of which can be found in papers by Park [1988; 1989; 1991], Lee [1985], and Gnoffo et al. [1989]. In the two-temperature model of Park, the approximation is made that the internal energy states of air can be adequately described by two temperatures: one temperature provides a measure of the translational-rotational energies of the atoms and molecules and a second temperature describes the molecular vibrational and electron energy states. Although, in the more sophisticated three-temperature model of Lee, an additional temperature is introduced to represent separately the electron energies, in both of these models, the vibrational energies of all species are described by a single vibrational temperature of energy. The model of this appendix is a multivibrational-temperature one that utilizes a unique temperature (or energy) to describe the vibrational energy state of each polyatomic species. The justifications for the use of a single vibrational temperature in the two- and three-temperature thermodynamic models are three fold. Firstly, numerical evidence suggests that the differences in the vibrational temperatures of nitrogen and oxygen are small for some blunt-body flows. Secondly, the accuracy of multivibrational temperature models is limited by the reliability of available relaxation rate data. Finally, the two- and three-temperature models require the solution of fewer partial-differential equations and are therefore more tractable, particularly for complicated three-dimensional flow simulations. However, a number of the underlying assumptions and empirical models for the two- and three-temperature approximations remain to be fully verified and/or substantiated [Park, 1989].

C.3 Five-Species Four-Temperature Model

C.3.1 Dissociation-Recombination Reaction Mechanism

As indicated in the introduction, if temperatures remain less than approximately 8,000 K, the quantities of ionized species and free electrons are insignificant and the chemical composition of high-temperature air can be adequately described by considering the five species N\(_2\), O\(_2\), NO, N, and O [Bray, 1971; Vincenti and Kruger, 1975; Anderson, 1989]. In the present multivibrational-temperature model for air only these five species are included and the chemical reaction mechanism of the mixture is represented by the following elementary reactions:

\[
\begin{align*}
O_2 + M &\rightarrow 2O + M, \\
N_2 + M &\rightarrow 2N + M, \\
NO + M &\rightarrow N + O + M, \\
NO + O &\rightarrow N + O_2, \\
N_2 + O &\rightarrow NO + N,
\end{align*}
\]

(C.6)

where M is a collision partner or catalytic molecule; it can be any one of the five species.
Seventeen elementary reactions (fifteen dissociation/recombination and two exchange reactions) are represented by the reaction scheme of Eq. (C.6). The forward reactions of the first three reaction equations above are bimolecular dissociation reactions (reactions involving the collision of two molecules) and the associated reverse reactions are termolecular recombination reactions (reactions involving the collision of three molecules). The forward and reverse reactions of the fourth and fifth reaction equations are bimolecular exchange or shuffle reactions involving NO. The forward exchange reactions are fast compared with the dissociation reactions and are important in establishing the concentrations of NO and N in many flow situations. It is interesting to note that the reaction

\[ \text{N}_2 + \text{O}_2 = 2\text{NO}, \quad (\text{C.7}) \]

was included in reaction mechanisms of air in many early chemical nonequilibrium flow studies; however, it is now known that this reaction does not take place directly through bimolecular collisions of \( \text{N}_2 \) and \( \text{O}_2 \) [Bray, 1971]. Instead, the production of nitric oxide from nitrogen and oxygen actually occurs through a complex process involving the elementary reactions of Eq. (C.6).

### C.3.2 Chemical Rate Equations

Collision theory and the law of mass action (backed by considerable experimental evidence) may be used to describe the finite-rate processes of the aforementioned reaction mechanism and thereby provide empirical expressions for the net time rate of change of the species concentrations \( c_s \). These expressions take the form [Vincenti and Kruger, 1975; Anderson, 1982; Anderson, 1989]

\[ w_s = \frac{M_s}{\rho} \sum_{r=1}^{N_R} \left( \sigma_{s,r}^b - \sigma_{s,r}^f \right) \left\{ k_r^f \prod_{s' = 1}^{N} \left( \frac{c_{s'}^{f} \rho}{M_{s'}} \right) \sigma_{s',r}^f - k_r^b \prod_{s' = 1}^{N} \left( \frac{c_{s'}^{b} \rho}{M_{s'}} \right) \sigma_{s',r}^b \right\}, \quad (\text{C.8}) \]

where \( \sigma_{s,r}^f \) and \( \sigma_{s,r}^b \) are the stoichiometric coefficients of the reactant and product species \( s \) of reaction \( r \), \( k_r^f \) and \( k_r^b \) are the forward and backward reaction rates of reaction \( r \), and \( M_s \) is the molecular weight of species \( s \). The variable \( N_R \) represents the total number of elementary reactions. In this case \( N_R = 17 \). Note that the forward and reverse reaction rates can be related by the equation

\[ k_r^{eq} = \frac{k_r^f}{k_r^b}, \quad (\text{C.9}) \]

where \( k_r^{eq} \) is the equilibrium constant for the reaction \( r \).

In general, the reaction rates \( k_r^f \) and \( k_r^b \) are temperature dependent and can be prescribed by modified forms of the Arrhenius equation. They can be written as

\[ k_r^f = C_r^f T_r^{n_f^f} \exp \left( \frac{-E_f^f}{K T_r} \right), \quad k_r^b = C_r^b T_r^{n_b^b} \exp \left( \frac{-E_b^b}{K T_r} \right), \quad (\text{C.10}) \]

where \( K \) is Boltzmann’s constant, \( C_r^f \), \( C_r^b \), \( n_f^f \), \( n_b^b \), \( E_f^f \), and \( E_b^b \) are the reaction rate coefficients (\( E_f^f \) and \( E_b^b \) are often referred to as activation energies), and \( T_r \) is the rate controlling temperature for the reaction \( r \). For the present model, chemical-vibrational coupling is neglected and the rate controlling temperature is assumed to be the translational-rotational...
Table C.1: Chemical Reaction Rate Coefficients of Dunn and Kang [1973].

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$C_i^f$</th>
<th>$n_i^f$</th>
<th>$E_i^f/K$</th>
<th>$C_i^b$</th>
<th>$n_i^b$</th>
<th>$E_i^b/K$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_2 + N \Rightarrow 2O + N$</td>
<td>$3.6 \times 10^{18}$</td>
<td>-1.0</td>
<td>$5.95 \times 10^4$</td>
<td>$3.0 \times 10^{15}$</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>$O_2 + NO \Rightarrow 2O + NO$</td>
<td>$3.6 \times 10^{18}$</td>
<td>-1.0</td>
<td>$5.95 \times 10^4$</td>
<td>$3.0 \times 10^{15}$</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>$O_2 + O \Rightarrow 3O$</td>
<td>$9.0 \times 10^{19}$</td>
<td>-1.0</td>
<td>$5.95 \times 10^4$</td>
<td>$7.5 \times 10^{16}$</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>$2O_2 = 2O + O_2$</td>
<td>$3.24 \times 10^{19}$</td>
<td>-1.0</td>
<td>$5.95 \times 10^4$</td>
<td>$2.7 \times 10^{16}$</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>$O_2 + N_2 = 2O + N_2$</td>
<td>$7.2 \times 10^{18}$</td>
<td>-1.0</td>
<td>$5.95 \times 10^4$</td>
<td>$6.0 \times 10^{15}$</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>$N_2 + O = 2N + O$</td>
<td>$1.9 \times 10^{17}$</td>
<td>-0.5</td>
<td>$1.13 \times 10^5$</td>
<td>$1.1 \times 10^{16}$</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>$N_2 + NO = 2N + NO$</td>
<td>$1.9 \times 10^{17}$</td>
<td>-0.5</td>
<td>$1.13 \times 10^5$</td>
<td>$1.1 \times 10^{16}$</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>$N_2 + O_2 \Rightarrow 2N + O_2$</td>
<td>$1.9 \times 10^{17}$</td>
<td>-0.5</td>
<td>$1.13 \times 10^5$</td>
<td>$1.1 \times 10^{16}$</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>$N_2 + N \Rightarrow 3N$</td>
<td>$4.08 \times 10^{22}$</td>
<td>-1.5</td>
<td>$1.13 \times 10^5$</td>
<td>$2.27 \times 10^{21}$</td>
<td>-1.5</td>
<td>0</td>
</tr>
<tr>
<td>$2N_2 = 2N + N_2$</td>
<td>$4.7 \times 10^{17}$</td>
<td>-0.5</td>
<td>$1.13 \times 10^5$</td>
<td>$2.72 \times 10^{16}$</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>NO + O_2 = N + O + O_2</td>
<td>$3.9 \times 10^{20}$</td>
<td>-1.5</td>
<td>$7.55 \times 10^4$</td>
<td>$1.0 \times 10^{20}$</td>
<td>-1.5</td>
<td>0</td>
</tr>
<tr>
<td>NO + N_2 = N + O + N_2</td>
<td>$3.9 \times 10^{20}$</td>
<td>-1.5</td>
<td>$7.55 \times 10^4$</td>
<td>$1.0 \times 10^{20}$</td>
<td>-1.5</td>
<td>0</td>
</tr>
<tr>
<td>NO + O = N + 2O</td>
<td>$7.8 \times 10^{20}$</td>
<td>-1.5</td>
<td>$7.55 \times 10^4$</td>
<td>$2.0 \times 10^{20}$</td>
<td>-1.5</td>
<td>0</td>
</tr>
<tr>
<td>NO + N = 2N + O</td>
<td>$7.8 \times 10^{20}$</td>
<td>-1.5</td>
<td>$7.55 \times 10^4$</td>
<td>$2.0 \times 10^{20}$</td>
<td>-1.5</td>
<td>0</td>
</tr>
<tr>
<td>2NO = N + O + NO</td>
<td>$7.8 \times 10^{20}$</td>
<td>-1.5</td>
<td>$7.55 \times 10^4$</td>
<td>$2.0 \times 10^{20}$</td>
<td>-1.5</td>
<td>0</td>
</tr>
<tr>
<td>NO + O = N + O_2</td>
<td>$3.2 \times 10^{20}$</td>
<td>1.0</td>
<td>$1.97 \times 10^4$</td>
<td>$1.3 \times 10^{10}$</td>
<td>1.0</td>
<td>$3.58 \times 10^2$</td>
</tr>
<tr>
<td>N_2 + O = NO + N</td>
<td>$7.0 \times 10^{18}$</td>
<td>0.0</td>
<td>$3.8 \times 10^4$</td>
<td>$1.56 \times 10^{13}$</td>
<td>0.0</td>
<td>0</td>
</tr>
</tbody>
</table>

temperature $T$ for all of the seventeen reactions (i.e., $T_r = T$).

The reaction rate coefficients $C_i^f$, $C_i^b$, $n_i^f$, $n_i^b$, $E_i^f$, and $E_i^b$ of Eq. (C.10) are generally determined from experimental observations. There are several sets of complete reaction-rate coefficient data for air available in the literature (e.g., [Dunn and Kang, 1973; Park, 1988; Park, 1989; Gnooffo et al., 1989; Mitcheltree, 1991; Sagnier and Marraffa, 1991]); however, for the purposes of the present work, the data set compiled by Dunn and Kang [1973] is used. Although it can be shown that equilibrium constants $k_r^q$ derived from the rate constants of Dunn and Kang via Eq. (C.9) are incorrect at temperatures above 10,000 K [ Mitcheltree, 1991], the data set appears to be reasonable for temperatures up to 8,000 K (the data set was compiled from experimental data taken at temperatures below 12,000 K) and has been used in a number of nonequilibrium flow studies. The chemical rate coefficients of Dunn and Kang for the seventeen reactions of interest are tabulated in Table C.1. Note that $k_i^f$ and $k_i^b$ have units of cm$^3$·mole$^{-1}$·s$^{-1}$ for bimolecular reactions and cm$^6$·mole$^{-2}$·s$^{-1}$ for termolecular reactions when the constants of Table C.1 are used in the reaction rate expressions of Eq. (C.10).

### C.3.3 Heats of Formation

In order to calculate the total change in the zero-point energy of the air mixture resulting from ongoing chemical reactions, values for the heats of formation $\Delta h_i^0$ are required. The heats of formation of the five species N$_2$, O$_2$, NO, N, and O are listed in Table C.2. These values are taken from the JANAF thermochemical tables [Chase et al., 1985] and are used in the present thermochemical nonequilibrium model.
Table C.2: Heats of Formation $\Delta h^0_f$.

<table>
<thead>
<tr>
<th>Species</th>
<th>$\Delta h^0_f$ (kJ/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N$_2$</td>
<td>0.00</td>
</tr>
<tr>
<td>O$_2$</td>
<td>0.00</td>
</tr>
<tr>
<td>NO</td>
<td>2,991.89</td>
</tr>
<tr>
<td>N</td>
<td>33,613.91</td>
</tr>
<tr>
<td>O</td>
<td>15,424.95</td>
</tr>
</tbody>
</table>

C.3.4 Vibrational Rate Equations

The finite-rate relaxation of the vibrationally excited diatomic molecules N$_2$, O$_2$, and NO is represented in the five-species four-temperature model by assuming that they behave as ideal harmonic oscillators. It follows from this assumption that, under conditions of thermal dynamic equilibrium, the equilibrium vibrational energy $e^*_v_s$ of species $s$ can be related to the translational-rotational temperature $T$ and defined by

$$e^*_v_s = \frac{\Theta_{v_s} R_s}{\exp(\Theta_{v_s}/T) - 1},$$  \hspace{1cm} (C.11)

where $\Theta_{v_s}$ is the characteristic vibrational temperatures of the species. In this work, values for $\Theta_{v_{N_2}}$, $\Theta_{v_{O_2}}$, and $\Theta_{v_{NO}}$ are taken to be 3353, 2239, and 2699 K, respectively [Barrow, 1962]. It is then further assumed that the relaxation process from an excited nonequilibrium state to a state of thermodynamic equilibrium occurs only through translational-vibrational collisions (i.e., collisions in which there is energy exchange between the translational and vibrational modes) and vibrational-vibrational collisional effects are not considered. Therefore, the time rate of change of the vibrational energy $e_{v_s}$ of the species $s$ may be prescribed by the rate equation [Vincenti and Kruger, 1975; Anderson, 1982; Anderson, 1989]

$$q_s = \frac{e^*_v_s - e_{v_s}}{\tau_s},$$  \hspace{1cm} (C.12)

where $\tau_s$ is the characteristic relaxation time. This rather simple vibrational rate equation, sometimes called the Landau-Teller law, states that, at any given instant, the rate at which the vibrational energy of a given species $s$ approaches the equilibrium energy is directly proportional to the difference between the equilibrium value and the current nonequilibrium value. If, as is often done, one now assumes that the nonequilibrium distribution of the energy states of the harmonic oscillators (diatomic molecules) is in fact a Boltzmann distribution characterized by a nonequilibrium vibrational temperature $T_v$, such that

$$e_{v_s} = \frac{\Theta_{v_s} R_s}{\exp(\Theta_{v_s}/T_v) - 1},$$  \hspace{1cm} (C.13)

then, when thermal equilibrium is achieved, $T = T_{v_{N_2}} = T_{v_{O_2}} = T_{v_{NO}}$. Note that although the vibrational temperatures defined by Eq. (C.13) are useful measures of thermal nonequilibrium, they should be used with caution because, in general, the nonequilibrium distribution
of vibrational energy states cannot be represented by a Boltzmann distribution. Note that
the effect of preferential dissociation of vibrationally excited diatomic molecules is not in­
cluded in the model and a value of unity is used for \( \beta_s \) in the vibrational energy equations
of Eq. (C.5).

To complete the modeling of the vibrational relaxation processes, expressions for the
characteristic relaxation times are required. The semi-empirical correlations of Millikan
and White [1963], based on modifications to the Landau-Teller equation, are used herein to
determine \( \tau_s \). These correlations have the form

\[
\tau_s = \frac{\sum_{s'} \frac{c_{s'}}{M_{s'}} \exp[A_s(T^{-1/3} - 0.015(\frac{M_s}{M_s + M_{s'}})^{1/4}) - 18.42]}{p \sum_{s'} \frac{c_{s'}}{M_{s'}}},
\]  

(C.14)

where \( A_{N_2} \), \( A_{O_2} \), and \( A_{NO} \) are taken to have values of 220, 129, and 168, respectively, and the
units of pressure, temperature, and molecular weight are atmospheres, Kelvin, and grams
per mole.

C.3.5 Chemical-Vibrational Coupling Effects

The chemical and vibrational rate equations described herein have been derived from theo­
retical considerations and analyses which do not encompass the coupling that is known to ex­
ist between the chemical reaction and vibrational relaxation processes. Chemical-vibrational
coupling (CVC) effects can be important, and both preferential CVC models (\( \beta_s = 1 \)) and
non-preferential CVC models (\( \beta_s > 1 \)) have been proposed [Treanor and Marrone, 1962;
Marrone and Treanor, 1963; Park, 1988; Park, 1989; Gnoffo et al., 1989]. In the CVC
model of Treanor and Marrone, the reaction rates are modified by a vibrational coupling
factor, whereas in other CVC models, the rate controlling temperature \( T_r \) for the reaction
\( r \) is taken to be a function of both the translational and vibrational temperatures \( T \) and
\( T_v \). Refer to the references given above for further details.

C.3.6 Ionization Effects

Finite-rate ionization is another physical phenomenon that is not modeled in the present
nonequilibrium analysis. For translational-rotational temperatures \( T \) exceeding 8,000 K,
ionization of the neutral molecules and atoms starts to increase and the concentration of
free electrons \( e^- \) becomes significant [Vincenti and Kruger, 1975; Anderson, 1982; Ander­
son, 1989]. Between the temperatures of 8,000 and 9,000 K, the dominant reaction that
characterizes the ionization rate processes of air is

\[
N + O \rightarrow NO^+ + e^-.
\]  

(C.15)

The present model could be extended to include this ionization process through the incor­
poration of energy and concentration equations for the two species \( NO^+ \) and \( e^- \) and the
addition of Eq. (C.15) to the reaction mechanism of Eq. (C.6). However, for temperatures
above 9,000 K, more complicated chemical kinetic mechanisms must be considered. As
noted in the introduction of this appendix, eleven-species models involving \( N_2, O_2, NO, N,
O, N_2^+, O_2^+, NO^+, N^+, O^+, e^- \) are usually employed in these cases.
C.4 Concluding Remarks

A five-species four-temperature thermodynamic model for air has been described that incorporates both thermal and chemical nonequilibrium effects. It is felt that the model is reasonably accurate for temperatures up to 8,000 K. Although more sophisticated modeling is certainly possible, the thermodynamic model of this appendix is more than adequate for nonequilibrium flow solution algorithm development and evaluation purposes. Note that the model can be used to represent the flows of either pure oxygen or nitrogen by setting the mass concentrations of the other species to zero. Additionally, a one-temperature model for chemical nonequilibrium flow studies can readily be achieved by assuming thermal equilibrium and by letting $T = T_{vN_2} = T_{vO_2} = T_{vNO}$, with Eq. (C.11) providing expressions for the equilibrium vibrational energies of the diatomic species. A one-temperature model of this form was employed in the recent work of Slomski et al. [1990].
Appendix D

Two-Dimensional Generalized Curvilinear Grid Generation

D.1 Summary

A numerical technique for the generation of structured generalized curvilinear grids on two-dimensional spatial domains is described. The mesh generator makes use of a Poisson's equation mapping technique to relate the coordinates of the physical domain having curved boundaries to the Cartesian coordinates of an orthogonal computational domain. The grids can have arbitrary boundary shape and may be composed of several subgrids. The distribution (i.e., spacing), orthogonality, and skewness of the grid lines can be controlled by a combination of algebraic stretching functions, that control the distribution of the nodes on the subgrid boundaries, and by the specification of the source terms of the Poisson equation mapping, that control the relative positions and concentrations of the nodes making up the numerical mesh. The resulting grids may be used in numerical methods that require the smooth structured discretization of the spatial domain to solve two-dimensional planar and axisymmetric fluid flow problems. Some example grids are given.

D.2 Introduction

Most modern numerical algorithms in computational fluid dynamics (CFD) solve a given set of partial-differential equations (PDEs) and thereby obtain the values of various dependent variables at discrete locations of a discretized solution domain. The spatial coordinates (nodes) of the discretized domain form a numerical grid or mesh, and the generation of such a grid for use in a CFD technique can be crucial when solving flow problems with complex geometries.

Computational meshes may be classified into two broad, but rather distinct, categories. In general, grids are either structured or unstructured. Information relating the node points of structured grids, such as node arrangement, nearest neighbor, difference molecule, and/or integration cell information, is inherent to their framework (i.e., grid connectivity is implied), whereas for unstructured grids, this additional information must be supplied (e.g., node-element information must be provided in finite-element techniques). Unstructured grids have advantages over structured grids, in that complicated geometries can be more readily handled and solution adaptive gridding and/or mesh embedding techniques may be more easily and effectively implemented (grid points are concentrated only where they are needed). However, it is quite difficult and computationally expensive to apply higher-order
upwind or symmetric total-variation-diminishing (TVD) finite-difference or finite-volume solution procedures on unstructured meshes. Furthermore, the large matrix bandwidth of the linear systems of equations that often result and must ultimately be solved in the application of implicit time-stepping and/or Newton iteration solution techniques on unstructured mesh can place heavy burdens on available computational resources. In contrast, matrix bandwidths of solution methods on structured grids are greatly reduced and approximate factorization or alternating-direction implicit (ADI) techniques may be employed to further reduce the bandwidths.

In the TVD flux-differencing schemes of the present work, structured meshes are used. The governing equations are solved in an orthogonal transformed (or computational) coordinate system and the conserved and primitive flow variables in the physical domain are related to their counterparts in the computational space by means of a generalized coordinate transformation. This readily permits those upwind difference schemes derived for Cartesian coordinates to be applied to flow problems with arbitrary solution domain boundaries as well as facilitates the clustering of grid points in regions of large solution gradients or where large numerical errors are expected [Anderson et al., 1984; Thompson et al., 1985; Vinokur, 1974]. Moreover, this permits the use of approximate factorization in the proposed implicit solution schemes which thereby reduces the systems of linear equations that must be solved to block tridiagonal form. Care must be taken to ensure that the structured grids are smooth and that the rate-of-change of the grid spacing is controlled in order that higher-order accuracy is maintained in both physical and computational spaces. Further, control of grid spacing, orthogonality, and skewness, particularly near domain boundaries, is both desirable and advantageous [Anderson et al., 1984; Sorenson, 1980; Thompson et al., 1985].

Various techniques have been proposed for generating structured grids, including algebraic or geometric methods, complex variable or conformal mapping techniques, as well as elliptic and hyperbolic differential equation methods [Anderson et al., 1984]. The important features, advantages, and limitations of many of these techniques are developed and discussed in the book by Thompson et al. [1985]. For the purposes of the present numerical study, a Poisson-equation method is used based on the work of Steger and Sorenson [Steger and Sorenson, 1979; Sorenson, 1980]. This numerical algorithm automates grid point selection and provides a mapping from the physical domain to computational coordinate space. In addition, the grid spacing, orthogonality, and skewness can be controlled by a combination of various algebraic stretching functions that control the distribution of the nodes on the grid boundaries, and by the specification the inhomogeneous source terms of the Poisson-equation mapping that control the relative positions and concentrations of the grid points. The technique has been used successfully to generate two-dimensional generalized curvilinear grids with both C- and O-type topology about airfoils and other geometries [Sorenson, 1980]. Note that it is possible to extend the technique for use in three-dimensional applications, which may be of interest in future studies.

This appendix provides a fairly detailed description of the proposed Poisson-equation elliptic mesh generation technique used herein to produce two-dimensional structured grids. Included are descriptions of the related mathematical theory, algebraic stretching functions, node-control source terms, as well as the iterative numerical solution procedure for actually computing the grid point locations. A few example numerical grids are also presented in order to demonstrate the usefulness of the method.
D.3 Poisson-Equation Elliptic Grid Generator

D.3.1 Theoretical Development

In all differential-equation grid generation techniques, whether they be of elliptic or hyperbolic type, there is an assumed one-to-one mapping of the generalized curvilinear grid in physical space to a uniformly spaced Cartesian grid in computational space. In the two-dimensional case, the mapping of the physical coordinates \((x, y)\) to the generalized curvilinear coordinates \((\zeta, \eta)\) of a rectangular computational space can be written as

\[
\zeta = \zeta(x, y), \quad \eta = \eta(x, y), \quad (D.1)
\]

for \(\zeta_{\text{min}} \leq \zeta \leq \zeta_{\text{max}}\) and \(\eta_{\text{min}} \leq \eta \leq \eta_{\text{max}}\). See Figure D.1. Similarly, the inverse mapping is given by

\[
x = x(\zeta, \eta), \quad y = y(\zeta, \eta). \quad (D.2)
\]

Note that it is not a requirement of the mapping that the computational domain be rectangular as shown in Figure D.1. This is usually done for the sake of simplicity. In the present grid generation algorithm, the complete two-dimensional mesh can be composed of several subgrids, each having a its own mapping to a rectangular computational space. The grid topology for this case is illustrated in Figure D.2.

Having established these one-to-one mappings, the following differential expressions can be written relating spatial position changes in the two coordinate systems:

\[
dx = x_{\zeta} d\zeta + x_{\eta} d\eta, \quad dy = y_{\zeta} d\zeta + y_{\eta} d\eta, \quad (D.3)
\]

\[
d\zeta = \zeta_x dx + \zeta_y dy, \quad d\eta = \eta_x dx + \eta_y dy, \quad (D.4)
\]

where \(x_{\zeta} = \partial x / \partial \zeta, \quad x_{\eta} = \partial x / \partial \eta, \quad y_{\zeta} = \partial y / \partial \zeta, \quad y_{\eta} = \partial y / \partial \eta, \quad \zeta_x = \partial \zeta / \partial x, \quad \zeta_y = \partial \zeta / \partial y, \quad \eta_x = \partial \eta / \partial x, \quad \text{and} \quad \eta_y = \partial \eta / \partial y\) are the metrics of the coordinate transformation. Manipulation of Eqs. (D.3) and (D.4) leads to expressions for the transformation metrics \(\zeta_x, \zeta_y, \eta_x, \text{and} \eta_y\) in terms of the metrics \(x_{\zeta}, x_{\eta}, y_{\zeta}, \text{and} y_{\eta}.\) They are

\[
\zeta_x = \frac{y_{\eta}}{J}, \quad \zeta_y = -\frac{x_{\eta}}{J}, \quad \eta_x = -\frac{y_{\zeta}}{J}, \quad \eta_y = \frac{x_{\zeta}}{J}, \quad (D.5)
\]

where \(J = x_{\zeta} y_{\eta} - x_{\eta} y_{\zeta}\) is the Jacobian of the coordinate transformation. By using these preceding expressions and applying the chain rule, partial derivatives of any dependent variable \(\phi\) with respect to the independent variables \(x\) and \(y\) of the physical domain can then be expressed in terms of the corresponding partial derivatives with respect to the computational coordinates \(\zeta\) and \(\eta.\) For example,

\[
\frac{\partial \phi}{\partial x} = \zeta_x \frac{\partial \phi}{\partial \zeta} + \eta_x \frac{\partial \phi}{\partial \eta} = \frac{y_{\eta} \partial \phi}{J \partial \zeta} - \frac{y_{\zeta} \partial \phi}{J \partial \eta}, \quad (D.6)
\]

\[
\frac{\partial \phi}{\partial y} = \zeta_y \frac{\partial \phi}{\partial \zeta} + \eta_y \frac{\partial \phi}{\partial \eta} = -\frac{x_{\eta} \partial \phi}{J \partial \zeta} + \frac{x_{\zeta} \partial \phi}{J \partial \eta}. \quad (D.7)
\]

Higher-order derivatives can be evaluated in a similar fashion. In this way, the governing
PDEs of interest can be transformed and solved on a uniform grid in the computational or \((\zeta, \eta)\) plane. Note, it is important that the coordinate mapping be smooth (i.e., differentiable) so that the transformation metrics and other related derivatives are defined and can be evaluated everywhere in the solution domain.

Following others such as Steger and Sorenson [Steger and Sorenson, 1979; Sorenson, 1980], the basis of the grid generation technique using Poisson’s equation is to specify the desired grid point distribution on the boundary of the physical space and then let the coordinate mappings, and hence transformations, satisfy

\[
\zeta_{xx} + \zeta_{yy} = P(\zeta, \eta), \quad \eta_{xx} + \eta_{yy} = Q(\zeta, \eta),
\]

on the interior of the solution domain, where the source terms of the Poisson equations \(P\) and \(Q\) are forcing functions that affect node distribution. Using the results described above, these two equations can be transformed and rewritten in the computational space as follows:

\[
Ax\zeta_{\zeta} - 2Bx\zeta_\eta + Cx_\eta \eta = -J^2(x_\zeta P + x_\eta Q), \quad (D.9)
\]
\[
Ay\zeta_{\zeta} - 2By\zeta_\eta + Cy_\eta \eta = -J^2(y_\zeta P + y_\eta Q), \quad (D.10)
\]

where \(A = x_\zeta^2 + y_\zeta^2\), \(B = x_\zeta x_\eta + y_\zeta y_\eta\), and \(C = x_\eta^2 + y_\eta^2\). Solution of these elliptic PDEs in the computational space provides the \((x, y)\) coordinates of each mesh point in the physical space. In the general case, a numerical solution technique is required. Note that by choosing the \(x = x(\zeta, \eta)\) and \(y = y(\zeta, \eta)\) coordinate mapping so as to satisfy Eqs. (D.9) and (D.10) ensures that the mapping is one to one and the resulting meshes are smooth, as well as permits the gridding of relatively complicated geometries. From Eq. (D.8), it can be seen that large values for \(P\) increase the gradients of \(\zeta_x\) and \(\zeta_y\) and hence tend to cluster constant \(\zeta\) lines in the physical domain. Similarly, large values for \(Q\) cluster constant \(\eta\) lines in the physical space. It should also be fairly evident that \(P\) and \(Q\) must be chosen carefully to obtain desirable grids.

**D.3.2 Specification of Grid Point Distributions on Boundaries**

In the present method, Dirichlet boundary conditions are used for \(x\) and \(y\) on the \(\zeta = \zeta_{min}\), \(\zeta = \zeta_{max}\), \(\eta = \eta_{min}\), and \(\eta = \eta_{max}\) boundaries of each subgrid. The prescription of these boundary conditions is automated by the use of algebraic node distribution or stretching functions [Anderson et al., 1984], which permit greater control of grid point clustering and local mesh refinement.

As an example of this, consider the lower boundary of a rectangular subgrid in the computational domain given by \(\eta = \eta_{min}\). Let us assume that the boundary is a straight line segment in the physical space with end points \((x_{min}, y_0)\) and \((x_{max}, y_0)\), and grid point clustering is desired in the \(x\) direction. Along this curve, boundary values for the \((x, y)\) coordinates in terms of the curvilinear coordinates \((\zeta, \eta)\) are then specified as follows:

\[
x(\zeta, \eta_{min}) = x_{min} + \phi \left( \frac{\zeta - \zeta_{min}}{\zeta_{max} - \zeta_{min}} \right) (x_{max} - x_{min}), \quad \zeta_{min} \leq \zeta \leq \zeta_{max},
\]
\[
y(\zeta, \eta_{min}) = y_0, \quad \zeta_{min} \leq \zeta \leq \zeta_{max},
\]

D.4
where $\phi(z)$ is an algebraic stretching that controls the distribution of the grid points on the boundary. Various types of stretching functions may be used and some useful ones are described below. Similar node specification procedures can be adopted for more complicated curves in the physical domain and for each of the three other boundaries of the subgrid.

The grid point distribution functions $\phi(z)$ of Eq. (D.11) should be smooth and differentiable. Various algebraic functions are employed herein, depending on the flow geometry and desired grid. The simple linear function

$$\phi(z) = z,$$

produces a uniform mesh with no grid point clustering. A stretching function that clusters nodes near $z=0$ is often useful. The function

$$\phi(z) = \frac{(\sigma + 1) - (\sigma - 1) \left[ \frac{\sigma + 1}{\sigma - 1} \right]^{1-z}}{\left[ \frac{\sigma + 1}{\sigma - 1} \right]^{1-z} + 1},$$

(D.14)

given in the text of Anderson et al. [1984] can be used for this where $\sigma$ is a parameter that controls the amount of clustering with $1 < \sigma < \infty$. The clustering increases as $\sigma$ approaches unity. Another related and useful stretching function, also described in the text of Anderson et al. [1984], can be written as

$$\phi(z) = \frac{(\sigma + 2B) \left[ \frac{\sigma + 1}{\sigma - 1} \right]^{(z-B)/(1-B)} - \sigma + 2B}{(1 + 2B) \left\{ 1 + \left[ \frac{\sigma + 1}{\sigma - 1} \right]^{(z-B)/(1-B)} \right\}},$$

(D.15)

where again $1 < \sigma < \infty$ and the clustering increases as $\sigma$ approaches unity. The function of Eq. (D.15) affords equal mesh refinement near $z=0$ and $z=1$ for $B=1/2$ whereas, for $B=0$, the mesh is refined only near $z=1$. Another alternative function given by

$$\phi(z) = z_c \left\{ 1 + \frac{\sinh[\sigma(z - B)]}{\sinh[\sigma B]} \right\},$$

(D.16)

can be used to cluster grid points near $z=z_c$ where $B = \ln\{[1 + (e^\sigma - 1)z]/[1 + (e^{-\sigma} - 1)z]\}$ and $0 < \sigma < \infty$. In this case, a value of $\sigma = 0$ results in no stretching and the stretching increases with increasing values of $\sigma$. Finally, the trigonometric stretching functions

$$\phi(z) = \sin\left( \frac{\pi z}{2} \right),$$

(D.17)

and

$$\phi(z) = 1 - \cos\left( \frac{\pi z}{2} \right),$$

(D.18)

are often quite useful and may be utilized.
D.3.3 Specification of Source Terms

Having prescribed the grid points on the mesh boundaries, the forcing functions \( P \) and \( Q \) of Eqs. (D.9) and (D.10) must be selected to obtain the desired grid. A wide range of choices for \( P \) and \( Q \) are permitted with the various choices resulting in different grids. Setting \( P = Q = 0 \) reduces the coordinate transformations of Eq. (D.8) to Laplace equations and produces a basic grid. However, in most cases, the resulting grid is not satisfactory, particularly near boundaries where both grid point clustering and grid orthogonality are very often required. In the present grid generator, the ideas of Steger and Sorenson [Steger and Sorenson, 1979; Sorenson, 1980] have been extended and \( P \) and \( Q \) are defined on the computational domain of each subgrid (i.e., \( \zeta_{\min} \leq \zeta \leq \zeta_{\max}, \eta_{\min} \leq \eta \leq \eta_{\max} \)) as follows:

\[
P(\zeta, \eta) = \left[ p_b e^{-a(\eta-\eta_{\min})} + p_t e^{-b(\eta_{\max}-\eta)} + p_r e^{-A(\zeta-\zeta_{\min})} + p_r e^{-B(\zeta_{\max}-\zeta)} \right] f_{bl} f_{br} f_{tl} f_{tr}, \tag{D.19}
\]

\[
Q(\zeta, \eta) = \left[ q_b e^{-c(\eta-\eta_{\min})} + q_t e^{-d(\eta_{\max}-\eta)} + q_r e^{-C(\zeta-\zeta_{\min})} + q_r e^{-D(\zeta_{\max}-\zeta)} \right] f_{bl} f_{br} f_{tl} f_{tr}, \tag{D.20}
\]

where

\[
f_{bl} = 1 - e^{-E[(\zeta_{\min})^2+(\eta-\eta_{\min})^2]}^{1/2}, \quad f_{br} = 1 - e^{-E[(\zeta_{\max}-\zeta)^2+(\eta-\eta_{\min})^2]}^{1/2},
\]

\[
f_{tl} = 1 - e^{-E[(\zeta_{\min})^2+(\eta_{\max}-\eta)^2]}^{1/2}, \quad f_{tr} = 1 - e^{-E[(\zeta_{\max}-\zeta)^2+(\eta_{\max}-\eta)^2]}^{1/2}.
\]

The values of the functions \( p_b = p_b(\zeta) \) and \( q_b = q_b(\zeta) \) are defined by specified conditions at \( \eta = \eta_{\min} \). Similarly, \( p_t = p_t(\zeta) \) and \( q_t = q_t(\zeta) \) are defined by specified conditions at \( \eta = \eta_{\max} \), \( p_r = p_r(\eta) \) and \( q_r = q_r(\eta) \) are defined by specified conditions at \( \zeta = \zeta_{\min} \), and \( p_r = p_r(\eta) \) and \( q_r = q_r(\eta) \) are defined by specified conditions at \( \zeta = \zeta_{\max} \). The constants \( a, b, c, d, A, B, C, D, \) and \( E \) are all positive valued. By using the preceding expressions for \( P \) and \( Q \), the node spacings near all four subgrid boundaries (bottom, top, left, and right) can be controlled and orthogonality of the constant \( \zeta \) and constant \( \eta \) grid lines at the boundaries can be enforced. The values of \( p_b, q_b, p_t, q_t, p_r, q_r, p_r, \) and \( q_r \) control the spacing and orthogonality and the exponential damping functions determine the extent to which the conditions at the boundaries influence the node point distribution in the interior of the subgrid.

Along the \( \eta = \eta_{\min} \) (bottom) boundary and far from the two corners \( (\zeta_{\min}, \eta_{\min}) \) and \( (\zeta_{\max}, \eta_{\min}) \), it can be assumed that \( P(\zeta, \eta = \eta_{\min}) = p_b(\zeta) \) and \( Q(\zeta, \eta = \eta_{\min}) = q_b(\zeta) \). It then follows that

\[
p_b(\zeta) = \left[ \frac{y_\eta R_1 - x_\eta R_2}{J} \right]_{\eta = \eta_{\min}}, \quad q_b(\zeta) = \left[ \frac{x_\zeta R_2 - y_\zeta R_1}{J} \right]_{\eta = \eta_{\min}}, \tag{D.23}
\]

where \( R_1 \) and \( R_2 \) are given by

\[
R_1 = x_\zeta |_{\eta = \eta_{\min}} p_b + x_\eta |_{\eta = \eta_{\min}} q_b = -\left[ \frac{ax_\zeta - 2b x_\zeta \eta + \gamma x_\eta}{J^2} \right]_{\eta = \eta_{\min}}, \tag{D.24}
\]

\[
R_2 = y_\zeta |_{\eta = \eta_{\min}} p_b + y_\eta |_{\eta = \eta_{\min}} q_b = -\left[ \frac{ay_\zeta - 2b y_\zeta \eta + \gamma y_\eta}{J^2} \right]_{\eta = \eta_{\min}}. \tag{D.25}
\]

Similarly, for the \( \eta = \eta_{\max} \) (top) boundary, it can be shown that
\[ p_t(\zeta) = \left[ \frac{y_\eta R_3 - x_\eta R_4}{J} \right]_{\eta=\eta_{\text{max}}} , \quad q_t(\zeta) = \left[ \frac{x_\zeta R_4 - y_\zeta R_3}{J} \right]_{\eta=\eta_{\text{max}}} , \]  

(D.26)

with

\[ R_3 = x_\zeta|_{\eta=\eta_{\text{max}}} p_t + x_\eta|_{\eta=\eta_{\text{max}}} q_t = -\left[ \frac{\alpha x_\zeta \zeta - 2\beta x_\eta \eta + \gamma x_\eta \eta}{J^2} \right]_{\eta=\eta_{\text{max}}} , \]  

(D.27)

\[ R_4 = y_\zeta|_{\eta=\eta_{\text{max}}} p_t + y_\eta|_{\eta=\eta_{\text{max}}} q_t = -\left[ \frac{\alpha y_\zeta \zeta - 2\beta y_\eta \eta + \gamma y_\eta \eta}{J^2} \right]_{\eta=\eta_{\text{max}}} . \]  

(D.28)

For the \( \zeta = \zeta_{\text{min}} \) (left) and \( \zeta = \zeta_{\text{max}} \) (right) boundaries, similar relationships also hold. They are

\[ p_t(\eta) = \left[ \frac{y_\zeta R_5 - x_\zeta R_6}{J} \right]_{\zeta=\zeta_{\text{min}}} , \quad q_t(\eta) = \left[ \frac{x_\zeta R_6 - y_\zeta R_5}{J} \right]_{\zeta=\zeta_{\text{min}}} , \]  

(D.29)

where

\[ R_5 = x_\zeta|_{\zeta=\zeta_{\text{min}}} p_t + x_\eta|_{\zeta=\zeta_{\text{min}}} q_t = -\left[ \frac{\alpha x_\zeta \zeta - 2\beta x_\eta \eta + \gamma x_\eta \eta}{J^2} \right]_{\zeta=\zeta_{\text{min}}} , \]  

(D.30)

\[ R_6 = y_\zeta|_{\zeta=\zeta_{\text{min}}} p_t + y_\eta|_{\zeta=\zeta_{\text{min}}} q_t = -\left[ \frac{\alpha y_\zeta \zeta - 2\beta y_\eta \eta + \gamma y_\eta \eta}{J^2} \right]_{\zeta=\zeta_{\text{min}}} , \]  

(D.31)

and

\[ p_r(\eta) = \left[ \frac{y_\zeta R_7 - x_\zeta R_8}{J} \right]_{\zeta=\zeta_{\text{max}}} , \quad q_r(\eta) = \left[ \frac{x_\zeta R_8 - y_\zeta R_7}{J} \right]_{\zeta=\zeta_{\text{max}}} , \]  

(D.32)

where

\[ R_7 = x_\zeta|_{\zeta=\zeta_{\text{max}}} p_r + x_\eta|_{\zeta=\zeta_{\text{max}}} q_r = -\left[ \frac{\alpha x_\zeta \zeta - 2\beta x_\eta \eta + \gamma x_\eta \eta}{J^2} \right]_{\zeta=\zeta_{\text{max}}} , \]  

(D.33)

\[ R_8 = y_\zeta|_{\zeta=\zeta_{\text{max}}} p_r + y_\eta|_{\zeta=\zeta_{\text{max}}} q_r = -\left[ \frac{\alpha y_\zeta \zeta - 2\beta y_\eta \eta + \gamma y_\eta \eta}{J^2} \right]_{\zeta=\zeta_{\text{max}}} . \]  

(D.34)

Equations (D.23)-(D.34) provide expressions for calculating \( p_b, q_b, p_t, q_t, p_l, q_l, p_r, \) and \( q_r, \) and hence the source terms \( P \) and \( Q, \) in terms of the coordinate mappings \( x = x(\zeta, \eta) \) and \( y = y(\zeta, \eta) \) and their derivatives. If the distribution of the nodes on the four boundaries of the subgrid are prescribed, as discussed in the previous subsection, all of these terms are known, except for \( x_\eta, y_\eta, x_\zeta, y_\zeta, x_\eta, y_\eta, \) and \( y_\eta \) on the constant \( \eta \) (bottom and top) boundaries and \( x_\zeta, y_\zeta, x_\zeta, y_\zeta, x_\zeta, \) and \( y_\zeta \) on the constant \( \zeta \) (left and right) boundaries. Following the method of Sorenson [Sorenson, 1980], these values are obtained by specifying the node spacing and enforcing orthogonality at boundaries. For a given or specified node spacing \( \Delta s \) along the \( \eta = \eta_{\text{min}} \) boundary, Sorenson shows that orthogonality of the grid lines at this boundary can be enforced by letting

\[ x_\eta|_{\eta=\eta_{\text{min}}} = \left[ \frac{-\Delta s y_\zeta}{(x_\zeta^2 + y_\zeta^2)^{1/2}} \right]_{\eta=\eta_{\text{min}}} , \quad y_\eta|_{\eta=\eta_{\text{min}}} = \left[ \frac{\Delta s x_\zeta}{(x_\zeta^2 + y_\zeta^2)^{1/2}} \right]_{\eta=\eta_{\text{min}}} , \]  

(D.35)
where $\Delta s$ is the physical distance between the boundary node and first node away from the boundary along a constant $\zeta$ grid line. Values for $x_\zeta$ and $y_\zeta$ on the boundary can then be obtained by differentiating the expressions of Eq. (D.35) with respect to $\zeta$, i.e.,

$$
x_{\zeta|\eta=\eta_{\text{min}}} = \frac{\partial}{\partial \zeta} \left( x_{\eta|\eta=\eta_{\text{min}}} \right), \quad y_{\zeta|\eta=\eta_{\text{min}}} = \frac{\partial}{\partial \zeta} \left( y_{\eta|\eta=\eta_{\text{min}}} \right). \quad (D.36)
$$

Values for $x_{\eta}$ and $y_{\eta}$ may be obtained as part of a solution procedure for Eqs. (D.9) and (D.10) when determining the interior mesh points of the grid (see next subsection). Identical procedures can be applied at the other three boundaries using the expressions

$$
x_{\eta|\eta=\eta_{\text{max}}} = \left[ \frac{-\Delta s y_{\zeta}}{(x_\eta^2 + y_\eta^2)^{1/2}} \right]_{\eta=\eta_{\text{max}}}, \quad y_{\eta|\eta=\eta_{\text{max}}} = \left[ \frac{\Delta s x_{\zeta}}{(x_\eta^2 + y_\eta^2)^{1/2}} \right]_{\eta=\eta_{\text{max}}}, \quad (D.37)
$$

$$
x_{\zeta|\zeta=\zeta_{\text{min}}} = \left[ \frac{\Delta s y_{\eta}}{(x_\eta^2 + y_\eta^2)^{1/2}} \right]_{\zeta=\zeta_{\text{min}}}, \quad y_{\zeta|\zeta=\zeta_{\text{min}}} = \left[ \frac{-\Delta s x_{\eta}}{(x_\eta^2 + y_\eta^2)^{1/2}} \right]_{\zeta=\zeta_{\text{min}}}, \quad (D.38)
$$

$$
x_{\zeta|\zeta=\zeta_{\text{max}}} = \left[ \frac{\Delta s y_{\eta}}{(x_\eta^2 + y_\eta^2)^{1/2}} \right]_{\zeta=\zeta_{\text{max}}}, \quad y_{\zeta|\zeta=\zeta_{\text{max}}} = \left[ \frac{-\Delta s x_{\eta}}{(x_\eta^2 + y_\eta^2)^{1/2}} \right]_{\zeta=\zeta_{\text{max}}}, \quad (D.39)
$$

where $\Delta s$ is appropriately defined. This completes the specification of the grid point control functions $P$ and $Q$.

### D.3.4 Numerical Implementation

Given the grid point distributions on the subgrid boundaries and utilizing the source terms $P$ and $Q$ of the previous subsection, which provide node spacing control and grid orthogonality near the boundaries, the elliptic PDEs of Eqs. (D.9) and (D.10) can then be solved on each subgrid using a numerical procedure in order to obtain the complete two-dimensional mesh. Gauss-Seidel point-iterative relaxation methods are sufficiently adequate for solving these types of equations and a successive-over-relaxation (SOR) technique with under-relaxation applied to the source terms is employed in the present grid generation procedure. The method is outlined below.

Let $(x_{i,j}, y_{i,j})$ be the physical space coordinates of discrete nodes $(i, j)$ making up a given two-dimensional structured curvilinear mesh. Further, let $(\zeta_{i,j}, \eta_{i,j})$ be the corresponding grid point coordinates in the related uniform computational space with $\Delta \zeta = \Delta \eta = 1$. By assuming a one-to-one coordinate mapping between these two coordinate systems satisfying the Poisson equations of Eq. (D.8), and then approximating the spatial derivatives appearing in Eqs. (D.9) and (D.10) by standard centered-difference expressions, the following equations can be derived for the grid point coordinates in the physical space:

$$
x_{i,j} = \frac{1}{2(\alpha_{i,j} + \gamma_{i,j})} \left[ J_{i,j}^2 \left( x_{\zeta_{i,j}} P_{i,j} + x_{\eta_{i,j}} Q_{i,j} \right) + \alpha_{i,j} (x_{i+1,j} + x_{i-1,j}) + \gamma_{i,j} (x_{i,j+1} + x_{i,j-1}) - \frac{1}{2} \beta_{i,j} (x_{i+1,j+1} - x_{i+1,j-1} - x_{i-1,j+1} + x_{i-1,j-1}) \right], \quad (D.40)
$$

$$
y_{i,j} = \frac{1}{2(\alpha_{i,j} + \gamma_{i,j})} \left[ J_{i,j}^2 \left( y_{\zeta_{i,j}} P_{i,j} + y_{\eta_{i,j}} Q_{i,j} \right) + \alpha_{i,j} (y_{i+1,j} + y_{i-1,j}) + \gamma_{i,j} (y_{i,j+1} + y_{i,j-1}) \right]
$$

D.8
\[ \eta_{i,j} (y_{i,j+1} + y_{i,j-1}) - \frac{1}{2} \beta_{i,j} (y_{i+1,j+1} - y_{i+1,j-1} - y_{i-1,j+1} + y_{i-1,j-1}) \]  \hspace{1cm} (D.41)

Quite obviously these difference expressions for \( x_{i,j} \) and \( y_{i,j} \) are nonlinear and not explicit and an iterative solution technique is necessary. A Gauss-Seidel SOR scheme is proposed here with under-relaxation for the source terms \( P \) and \( Q \). This point-iterative procedure can be defined by the following steps:

Step 1. **Specification of grid point boundary distributions.** Grid point distributions on all subgrid boundaries are specified using algebraic stretching functions.

Step 2. **Computation of an initial estimate of grid point locations.** An initial guess or estimate of the interior grid point locations are obtained using the grid point distributions at the boundaries and a transfinite interpolation procedure. Transfinite interpolation is described by Thompson et al. [1985].

Step 3. **Determination of metric and derivative information at boundaries.** Utilizing Eqs. (D.37) and (D.37)-(D.39) and the specified grid point boundary distributions from step 1, along with specified values for the normal node spacing \( \Delta s \), values for the metrics \( x_\eta \) and \( y_\eta \) at \( \eta = \eta_{\text{min}} \) and \( \eta = \eta_{\text{max}} \) and the metrics \( x_\zeta \) and \( y_\zeta \) at \( \zeta = \zeta_{\text{min}} \) and \( \zeta = \zeta_{\text{max}} \) are computed for each subgrid. Boundary values for \( x_\zeta \), \( y_\zeta \), \( x_{\zeta\zeta} \), \( y_{\zeta\zeta} \), \( x_{\zeta\eta} \), \( y_{\zeta\eta} \), \( x_{\eta\zeta} \), \( y_{\eta\zeta} \), and \( J \) at \( \eta = \eta_{\text{min}} \) and \( \eta = \eta_{\text{max}} \) and for \( x_\zeta \), \( y_\zeta \), \( x_{\zeta\zeta} \), \( y_{\zeta\zeta} \), \( x_{\zeta\eta} \), \( y_{\zeta\eta} \), \( x_{\eta\zeta} \), \( y_{\eta\zeta} \), and \( J \) at \( \zeta = \zeta_{\text{min}} \) and \( \zeta = \zeta_{\text{max}} \) can then be determined using simple centered-difference expressions. All of these quantities remain unchanged throughout the SOR iterative solution procedure.

Step 4. **Evaluation of second-order derivatives at boundaries.** Using the latest or most recent grid point solution, values for the partial derivatives \( x_{\eta\eta} \) and \( y_{\eta\eta} \) evaluated at \( \eta = \eta_{\text{min}} \) and \( \eta = \eta_{\text{max}} \) and for \( x_{\zeta\zeta} \) and \( y_{\zeta\zeta} \) evaluated at \( \zeta = \zeta_{\text{min}} \) and \( \zeta = \zeta_{\text{max}} \) are computed by means of the following difference relations:

\[
\begin{align*}
x_{\eta\eta}|_{\eta=\eta_{\text{min}}} &= \frac{1}{2} (-7x_{i,j_{\text{min}}+1} + 8x_{i,j_{\text{min}}+1} - x_{i,j_{\text{min}}+2}) - 3 x_{\eta}|_{\eta=\eta_{\text{min}}} , \\
y_{\eta\eta}|_{\eta=\eta_{\text{min}}} &= \frac{1}{2} (-7y_{i,j_{\text{min}}+1} + 8y_{i,j_{\text{min}}+1} - y_{i,j_{\text{min}}+2}) - 3 y_{\eta}|_{\eta=\eta_{\text{min}}} , \\
x_{\eta\eta}|_{\eta=\eta_{\text{max}}} &= \frac{1}{2} (-7x_{i,j_{\text{max}}+1} + 8x_{i,j_{\text{max}}+1} - x_{i,j_{\text{max}}+2}) + 3 x_{\eta}|_{\eta=\eta_{\text{max}}} , \\
y_{\eta\eta}|_{\eta=\eta_{\text{max}}} &= \frac{1}{2} (-7y_{i,j_{\text{max}}+1} + 8y_{i,j_{\text{max}}+1} - y_{i,j_{\text{max}}+2}) + 3 y_{\eta}|_{\eta=\eta_{\text{max}}} , \\
x_{\zeta\zeta}|_{\zeta=\zeta_{\text{min}}} &= \frac{1}{2} (-7x_{i_{\text{min}},j} + 8x_{i_{\text{min}},j} - x_{i_{\text{min}},j+2}) - 3 x_{\zeta}|_{\zeta=\zeta_{\text{min}}} , \\
y_{\zeta\zeta}|_{\zeta=\zeta_{\text{min}}} &= \frac{1}{2} (-7y_{i_{\text{min}},j} + 8y_{i_{\text{min}},j} - y_{i_{\text{min}},j+2}) - 3 y_{\zeta}|_{\zeta=\zeta_{\text{min}}} , \\
x_{\zeta\zeta}|_{\zeta=\zeta_{\text{max}}} &= \frac{1}{2} (-7x_{i_{\text{max}},j} + 8x_{i_{\text{max}},j} - x_{i_{\text{max}},j+2}) + 3 x_{\zeta}|_{\zeta=\zeta_{\text{max}}} , \\
y_{\zeta\zeta}|_{\zeta=\zeta_{\text{max}}} &= \frac{1}{2} (-7y_{i_{\text{max}},j} + 8y_{i_{\text{max}},j} - y_{i_{\text{max}},j+2}) + 3 y_{\zeta}|_{\zeta=\zeta_{\text{max}}} ,
\end{align*}
\]

as given by Sorenson [1980].

D.9
Step 5. **Evaluation of node distribution functions \(P\) and \(Q\).** The functions \(p_b, q_b, p_t, q_t, p_l, q_l, p_r,\) and \(q_r\) are calculated by using Eqs. (D.23)–(D.34) and then the node distribution forcing functions \(P\) and \(Q\) are evaluated over the entire solution domain by employing Eqs. (D.19)–(D.22). To ensure numerical stability of the SOR procedure, an under-relaxation technique is required when updating the values of \(p_b, q_b, p_l, q_l, p_r, q_r,\) and \(q_r\). For example, the function \(p_b\) is updated at the \(k\)th iterative step by using the expression

\[
p_b^k = p_b^{k-1} + \frac{\delta p_b^k - p_b^{k-1}}{|p_b^k - p_b^{k-1}|} \min \left( \omega_{PQ} \left| \frac{p_b^k - p_b^{k-1}}{p_b^k - p_b^{k-1}} \right|, \frac{1}{2} \max(p_b^{k-1}, 1) \right),
\]

where \(\omega_{PQ}\) is the under-relaxation parameter \((0 < \omega_{PQ} < 1)\) and the superscript \(\tilde{k}\) indicates the updated value before under-relaxation is applied. Similar procedures are employed when updating the other functions.

Step 6. **Re-evaluation of grid point locations.** The coordinates of the grid points are re-evaluated by applying one step of the Gauss-Seidel point-interative relaxation procedure. Updated values for \(x_{i,j}\) and \(y_{i,j}\) at the \(k\)th iterative step are obtained using

\[
x_{i,j}^k = x_{i,j}^{k-1} + \omega_{xy} \left( x_{i,j}^k - x_{i,j}^{k-1} \right),
\]

\[
y_{i,j}^k = y_{i,j}^{k-1} + \omega_{xy} \left( y_{i,j}^k - y_{i,j}^{k-1} \right),
\]

where \(\omega_{xy}\) is the SOR parameter \((1 < \omega_{xy} < 1.8)\) and the superscript \(\tilde{k}\) indicates solution values obtained from Eqs. (D.40) and (D.41) using the latest solution information at each node.

Step 7. **Continuation of SOR iterative solution procedure.** Steps 4, 5, and 6 are repeated until a converged solution is attained.

Typically, the exponential decay parameters \(a, b, c, d, A, B, C, D,\) and \(E\) for the source terms \(P\) and \(Q\) have values between 0.10 and 0.70, \(\omega_{PQ} = 0.30\), and \(\omega_{xy} = 1.7\). A converged mesh solution is then usually obtained within 200–300 iterations of the SOR procedure.

### D.4 Example Two-Dimensional Grids

Two examples of structured grids generated by the elliptic differential-equation method of this appendix are now given in order to illustrate the technique's capabilities. The first example is a 96 × 96 mesh. It is comprised of a single subgrid containing 9216 points and would be suitable for solving symmetric two-dimensional flows over a circular cylinder. The grid is depicted in Figure D.3. The second example is a 314 × 104 mesh (33075 grid points) having three subgrids. It is shown in Figure D.4. This second grid was generated for computing high-speed planar flows at a compression corner with a 27° wedge angle.

It can be observed from Figures D.3 and D.4 that, in both cases, grid lines are relatively smooth and mesh cells formed by adjacent nodes do not exhibit excessive skewness. It is also evident that the various algebraic stretching functions provide control of node spacing in a smoothly varying manner. Finally, inspection of the two grids also reveals that, where it is
necessary or required, orthogonality of the grid lines can be obtained at the grid boundaries.

D.5 Concluding Remarks

A Poisson-equation mesh generation technique and associated Gauss-Seidel SOR solution procedure has been described for obtaining two-dimensional structured generalized curvilinear grids having planar or axisymmetric geometry. The method provides a smooth one-to-one mapping between physical and computational planes and permits the control of node spacing and orthogonality near boundaries. Extensions to the three-dimensional case are possible.
Figure D.1: Mapping of the physical coordinates \((x, y)\) to generalized curvilinear coordinates \((\zeta, \eta)\).

Figure D.2: Schematic of grid topology illustrating subgrids.
Figure D.3: The $96 \times 96$ computational grid.
Figure D.4: The $314 \times 104$ computational grid.
Appendix E

Bibliography


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E.3


E.5


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E.7


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This study is concerned with the numerical solution of high-speed nonequilibrium gaseous flows with strong shocks. The extension of modern total-variation-diminishing (TVD) shock-capturing schemes to include thermochemical nonequilibrium high-temperature effects is of primary interest. Partially-decoupled upwind-based TVD flux-difference split schemes for the solution of the conservation laws governing two-dimensional nonequilibrium vibrationally relaxing and chemically reacting flows of thermally-perfect gaseous mixtures are presented. Both time-split semi-implicit and factored implicit flux-limited TVD upwind schemes are described. A multigrid version of the fully implicit TVD scheme is also proposed for the more efficient computation of time-invariant solutions. A novel partially-decoupled flux-difference splitting approach is adopted. The fluid conservation laws and the finite-rate species concentration and vibrational energy equations are decoupled by means of a frozen flow approximation. The resulting partially-decoupled gas dynamic and thermodynamic subsystems are then integrated alternately in lagged manner within a two-stage time marching procedure, thereby providing explicit coupling between the two equations sets. Extensions of Roe's approximate Riemann solvers, giving the eigenvalues and eigenvectors of the fully coupled systems, are used to evaluate the numerical flux functions.

The predictive capabilities of the shock-capturing methods are demonstrated and their usefulness appraised, by solving a number of different flows with both complicated shock structure and complex nonlinear wave interactions. The problems considered include nonstationary oblique shock-wave reflections and diffractions and steady high-speed nozzle, compression ramp, and blunt-body flows. The numerical results are compared to available experimental data in many cases.

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